Bayesian Statistics
for
Effective Field Theories

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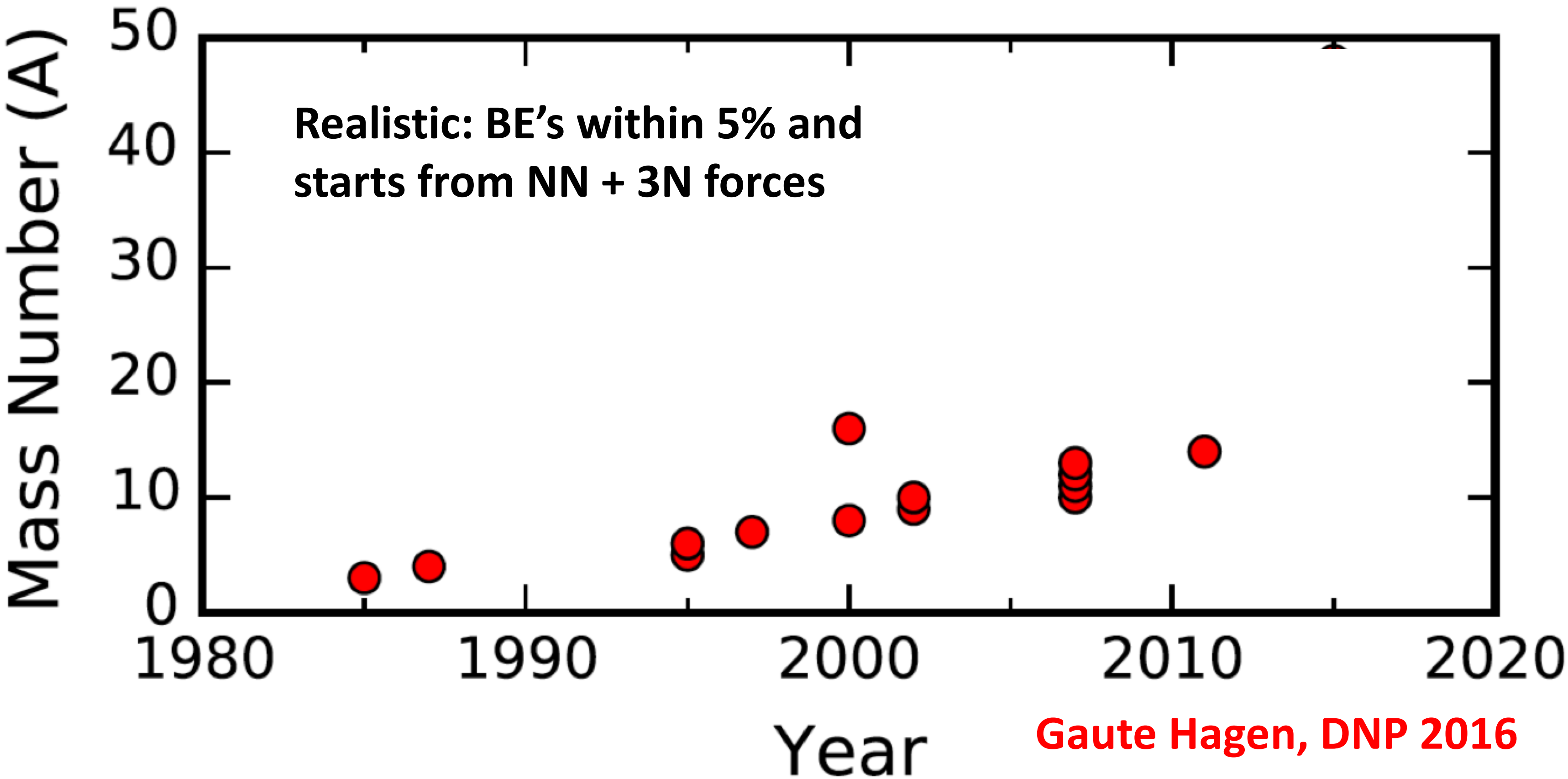
U.S. DEPARTMENT OF ENERGY

NSF

NUCLEI
Nuclear Computational Low-Energy Initiative

Ab initio calculations: The nuclear structure hockey stick



Gaute Hagen, DNP 2016

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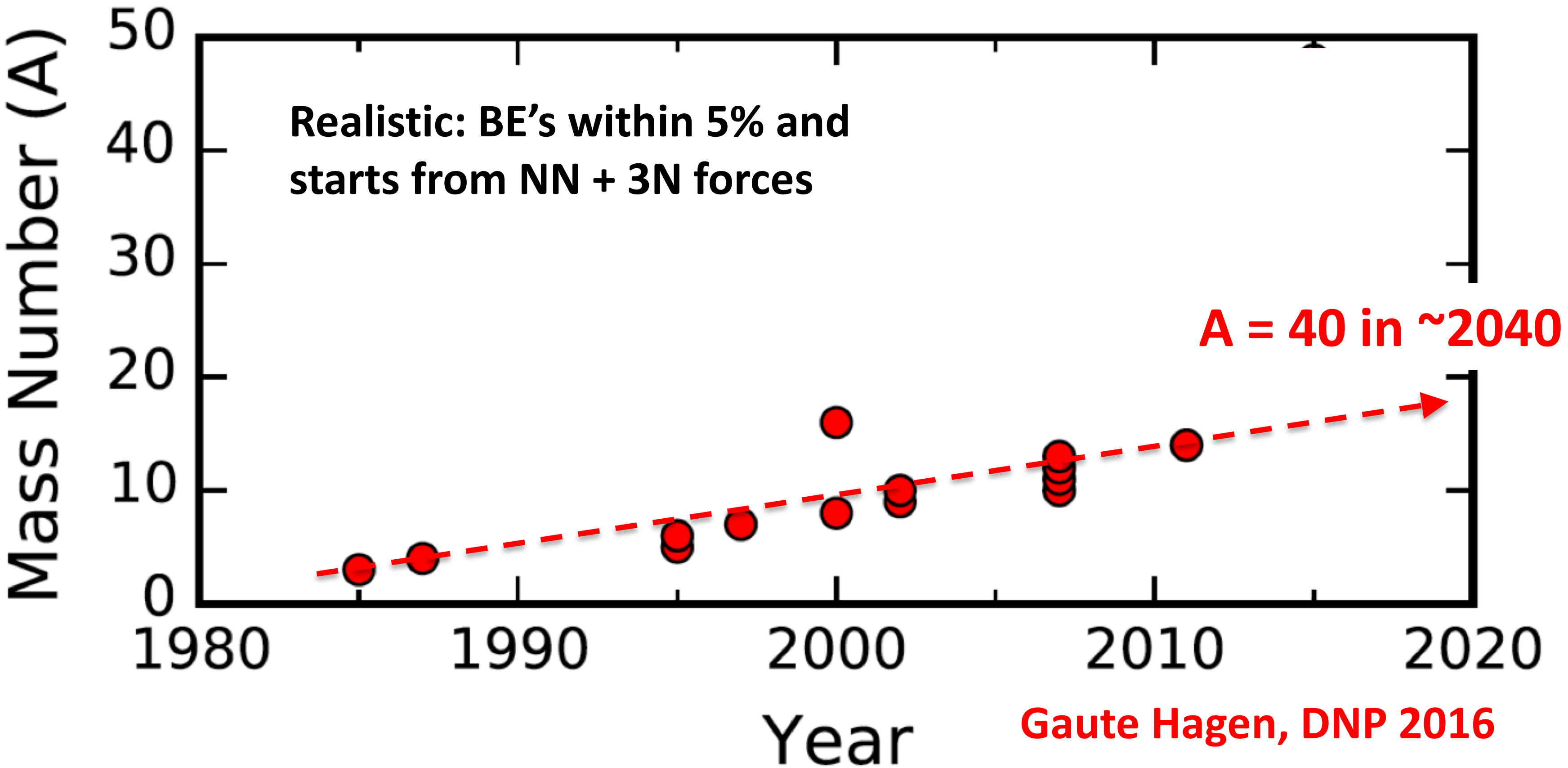

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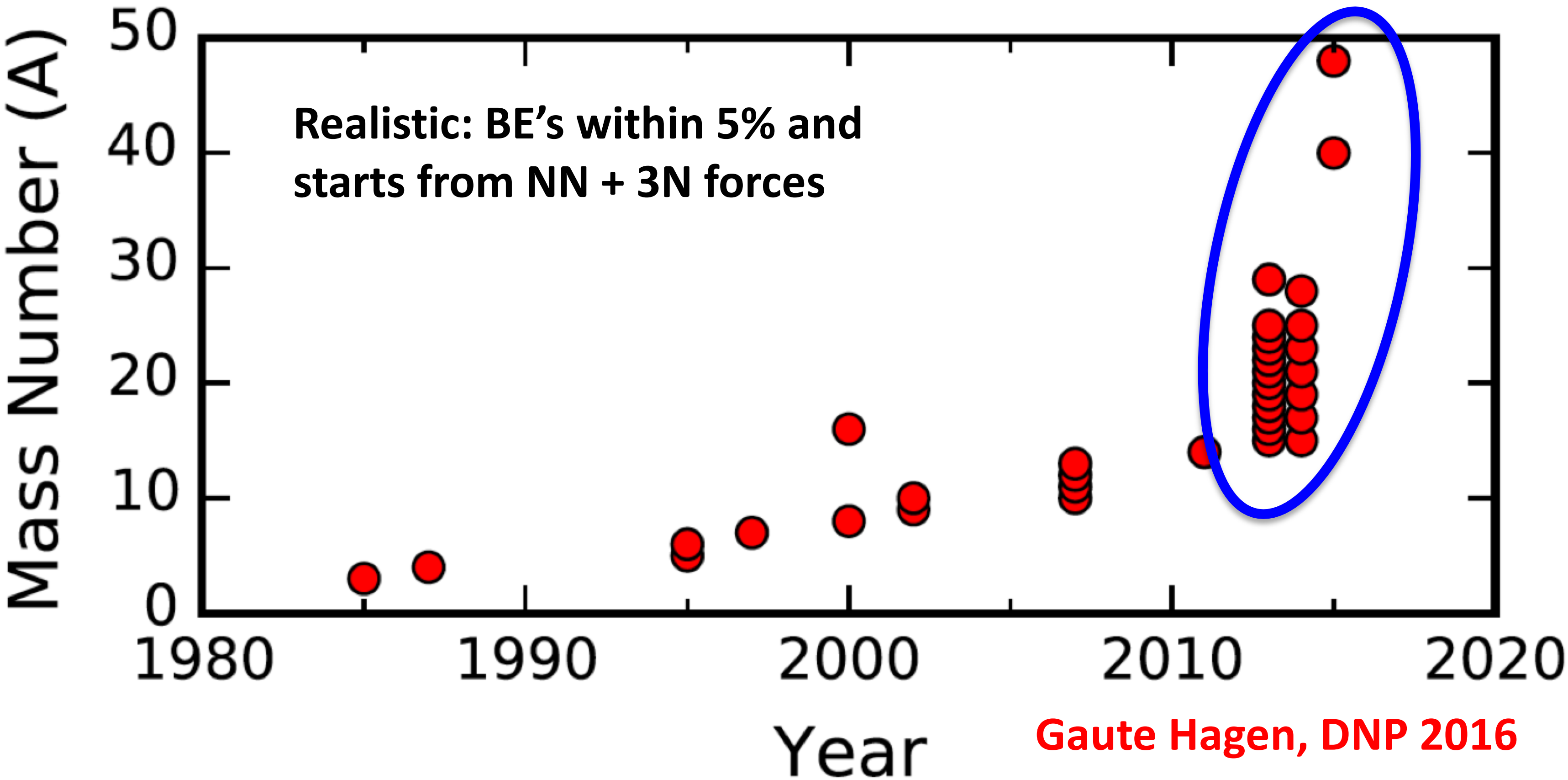

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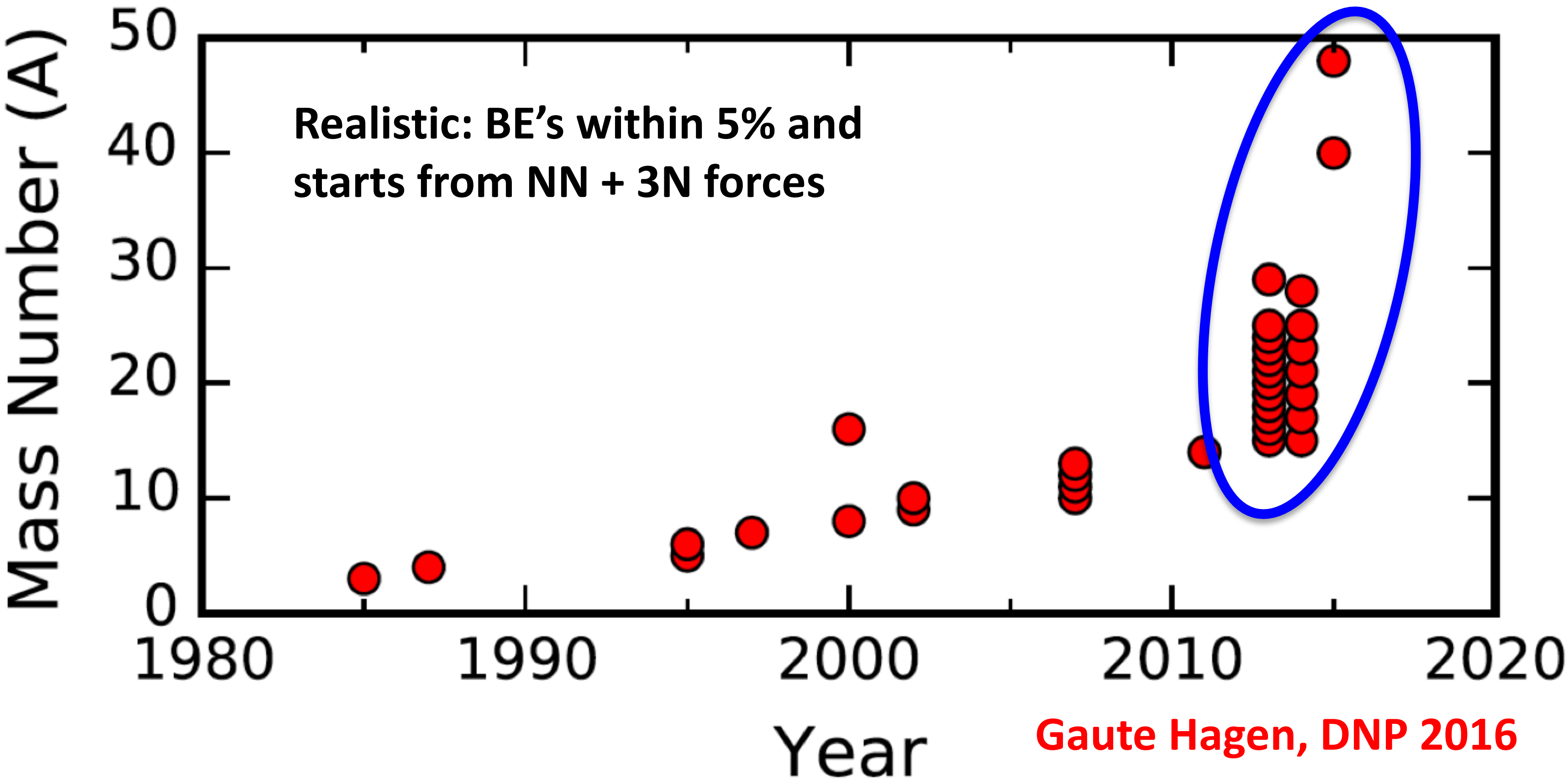
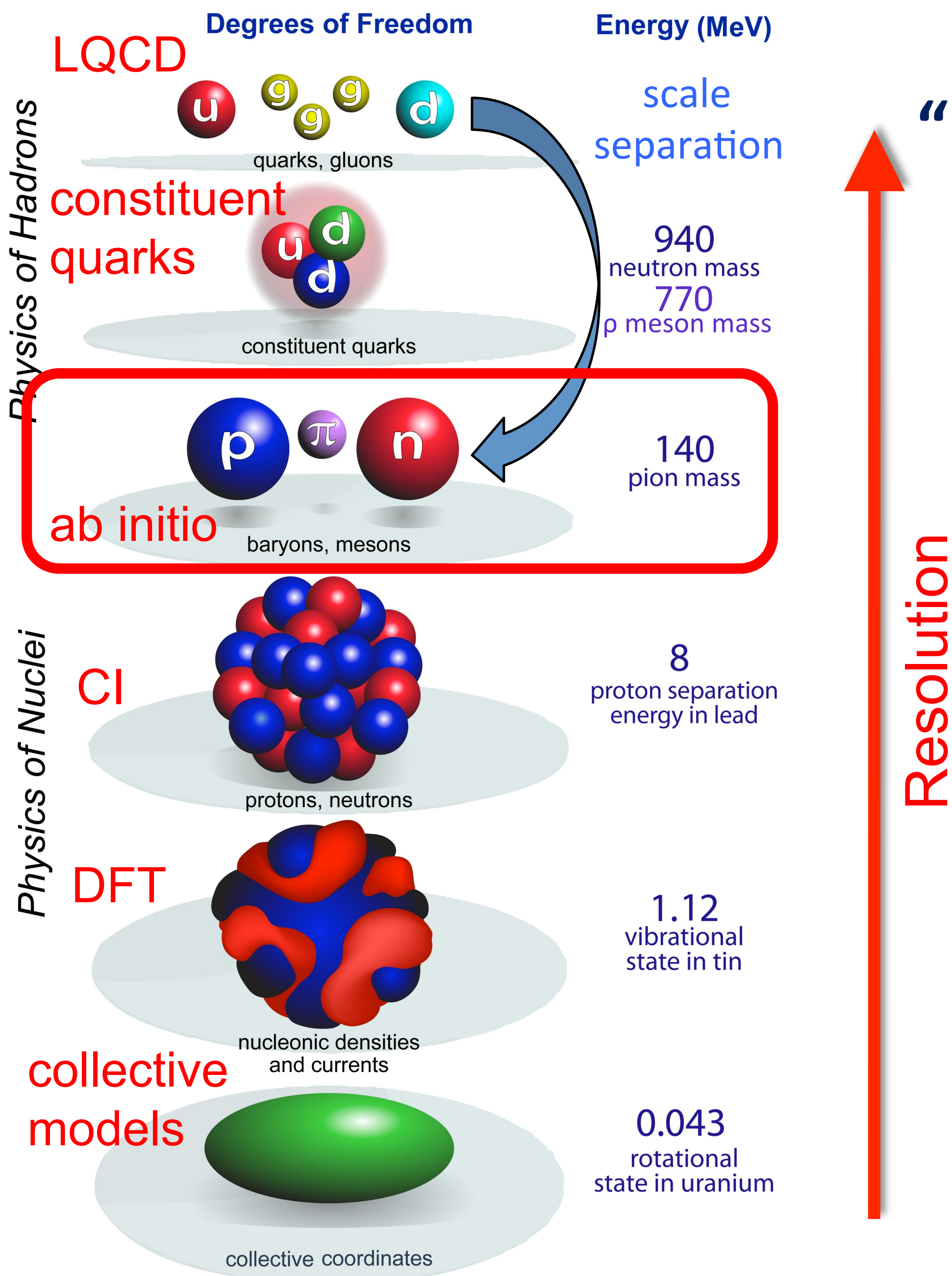


Gaute Hagen, DNP 2016

Why has the reach of these precision nuclear calculations increased?

- *Effective field theory* (EFT) and related techniques have enabled an explosion of new solution methods that grow polynomially with size
- **New challenge: robust and verifiable theoretical error estimates**

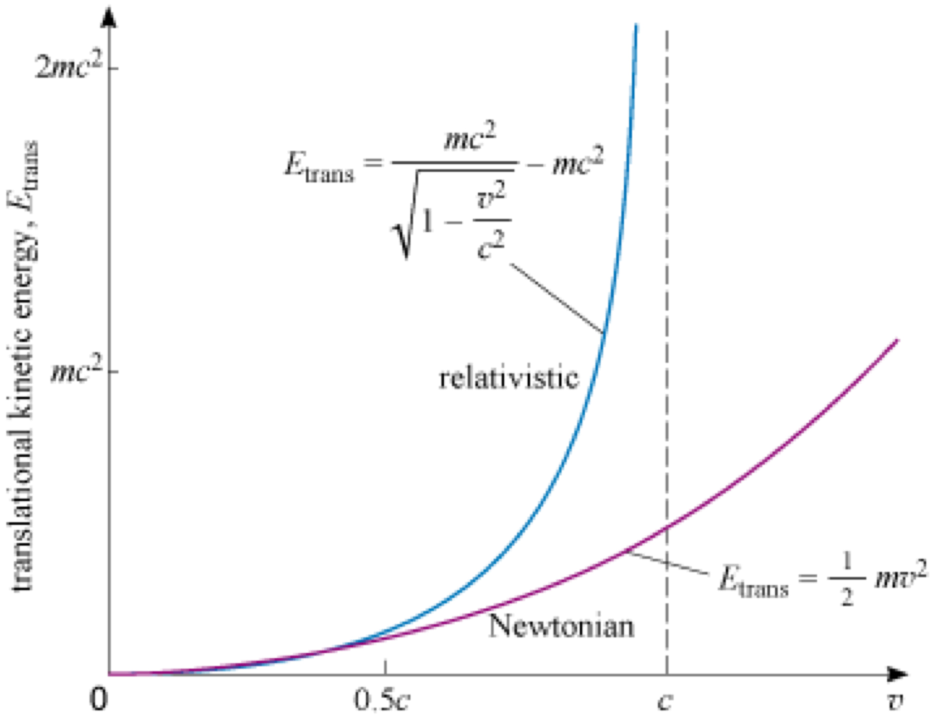
Tower of *emergent* phenomena in nuclear physics



"Effective field theory" (EFT)

- Systematic construction of nuclear forces used to make predictions
- Each order includes nontrivial functions; equations to be solved are highly nonlinear
- *Expectation* is that output results are expansions in a small parameter, but *not* a Taylor expansion

EFT and prior knowledge: A relativity Taylor-expansion analogy



Suppose Einstein didn't develop relativity. The kinetic energy $K(v^2)$ of an electron would still deviate from the Physics 101 formula. How would we determine it from measurements at small speed v?

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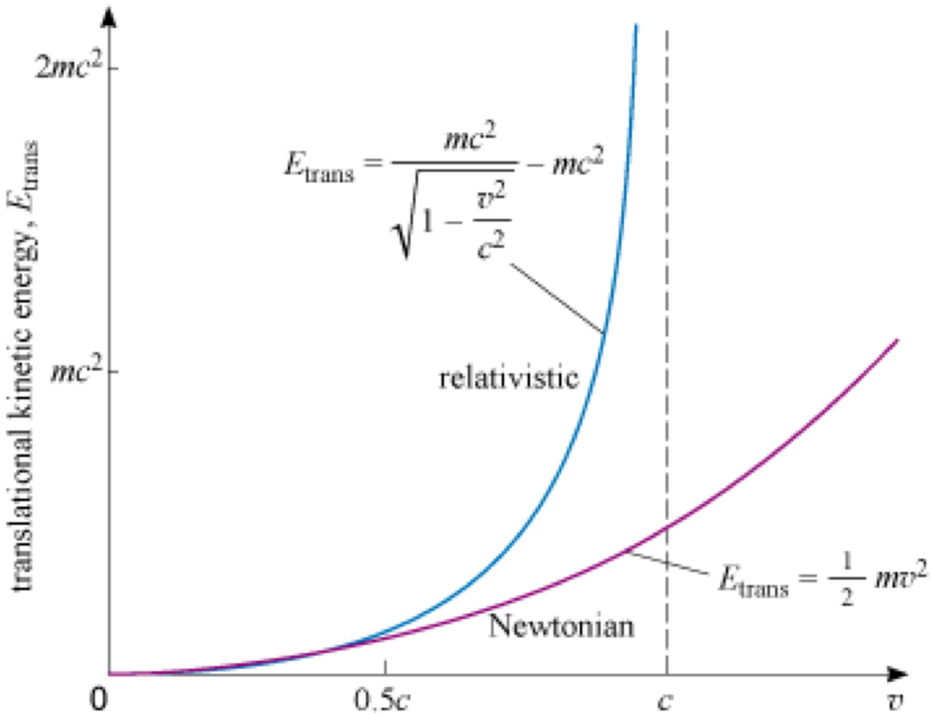

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Physics ⇒Taylor expansion in v^2 only:

$$K(v^2) \approx \frac{1}{2}mv^2[a_0 + a_2 v^2 + a_4 v^4 + \mathcal{O}(v^6)]$$

What do we know about the a_i?

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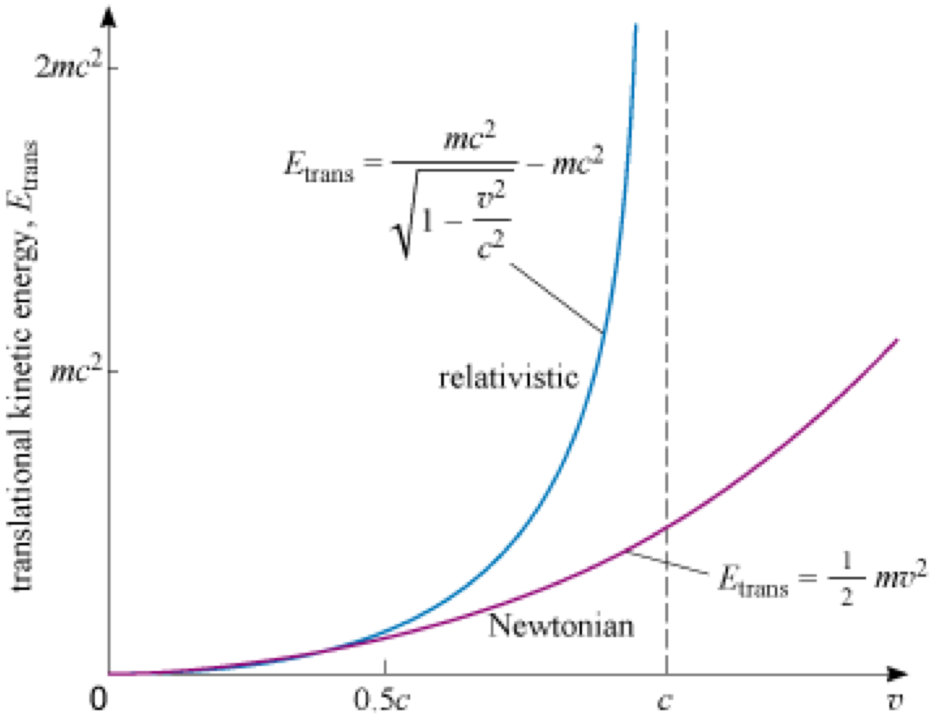

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What do we know about the a_i?

- Physics input: there is only one (unknown) scale of velocity in the problem; call it "c"

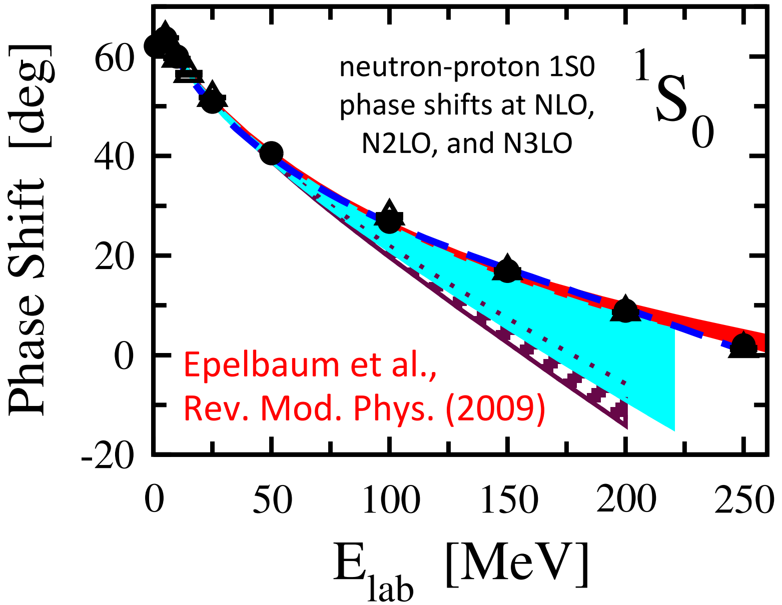
$$\Longrightarrow \;\; K(v^2) \approx \frac{1}{2}mv^2[b_0 + b_2(v/c)^2 + b_4(v/c)^4 + \mathcal{O}(1)(v/c)^6 + \cdots]$$

- The expectation is that the b_i are *natural*, meaning of order unity.
- We can check this case: $b_0 = 1$, $b_2 = 3/4$, $b_4 = 5/8$, $b_6 = 35/64$, … ⇒ natural!
- Model the discrepancy *coefficient*. Can we determine the breakdown scale c?

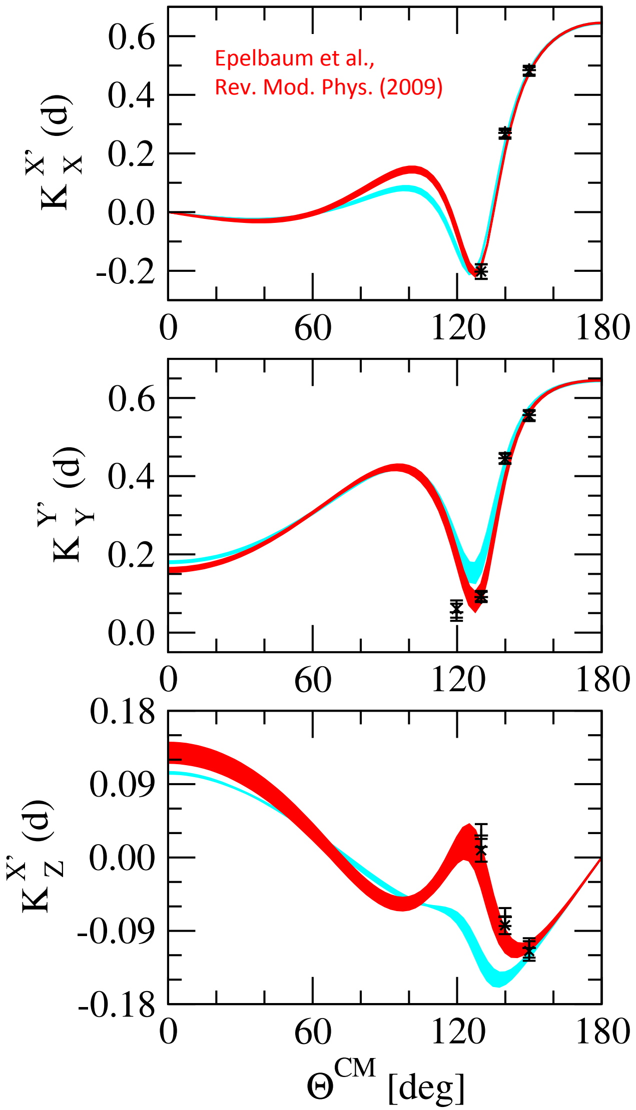
Previous UQ: Error bands in chiral EFT

Until recently, little examination of theoretical uncertainties (cf. experimental UQ), which are *systematic* errors

Previous work used EFT cutoff (regulator parameter) variation to determine bands:



chiral EFT predictions for p–d spin observables



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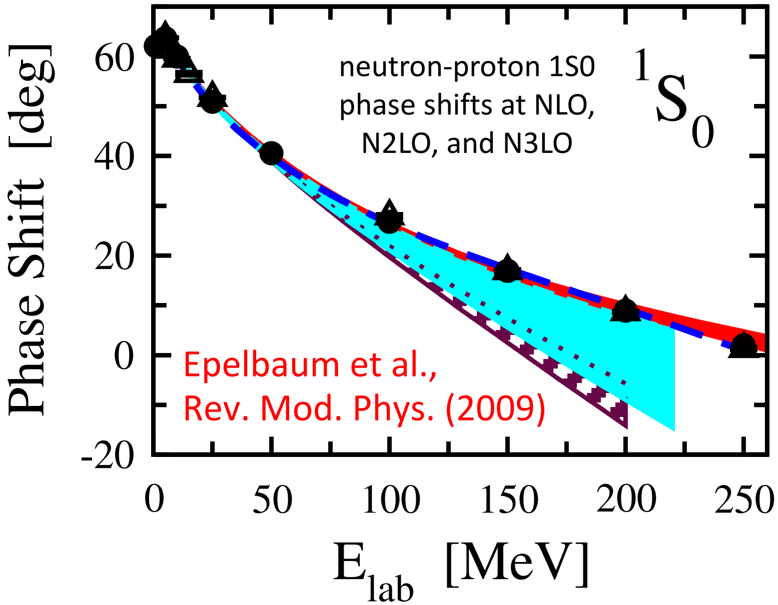

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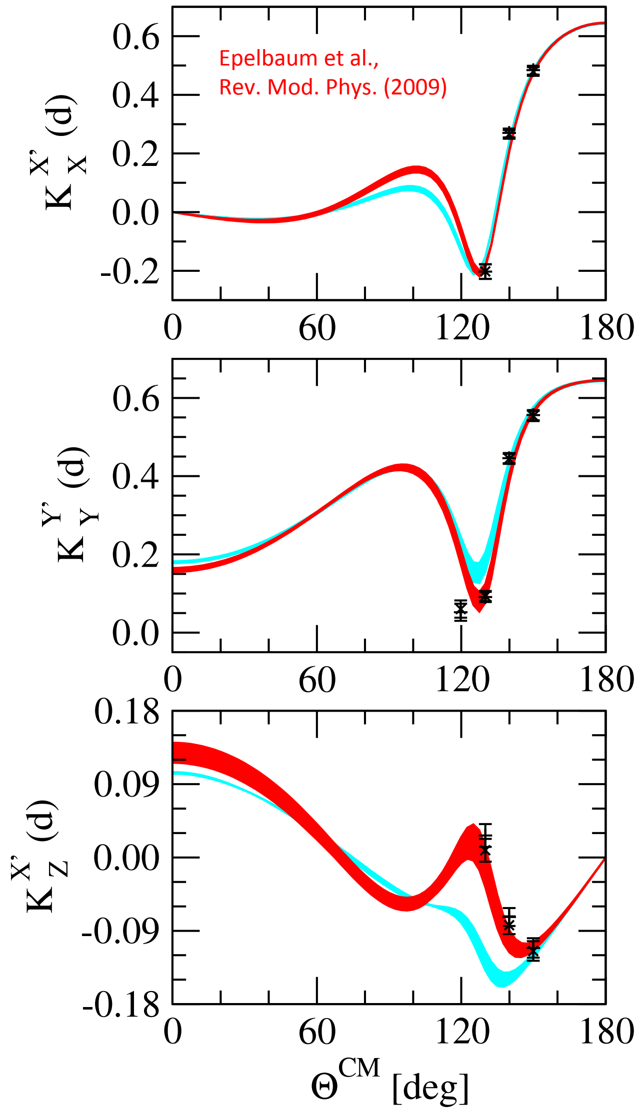

Problems with this as UQ (see right figure):

- unnatural systematics of bands
- often underestimates uncertainty
- statistical interpretation???
- Is the EFT actually working?

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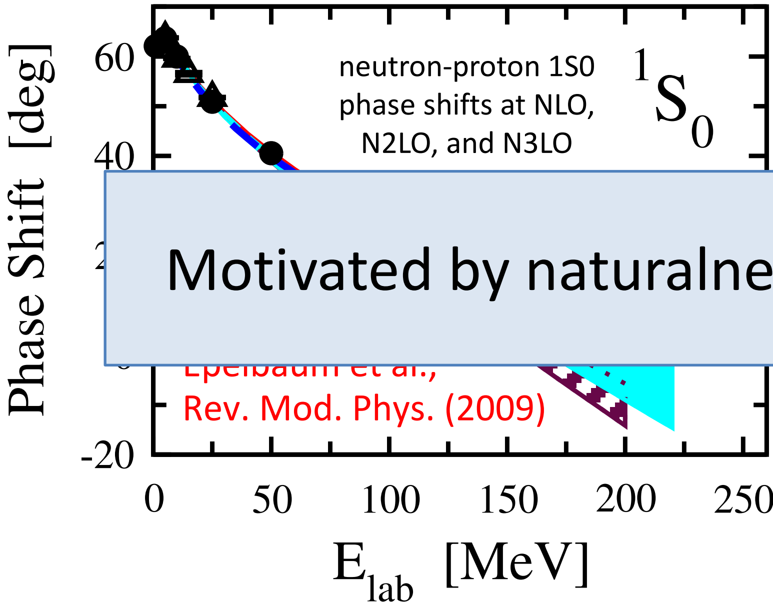

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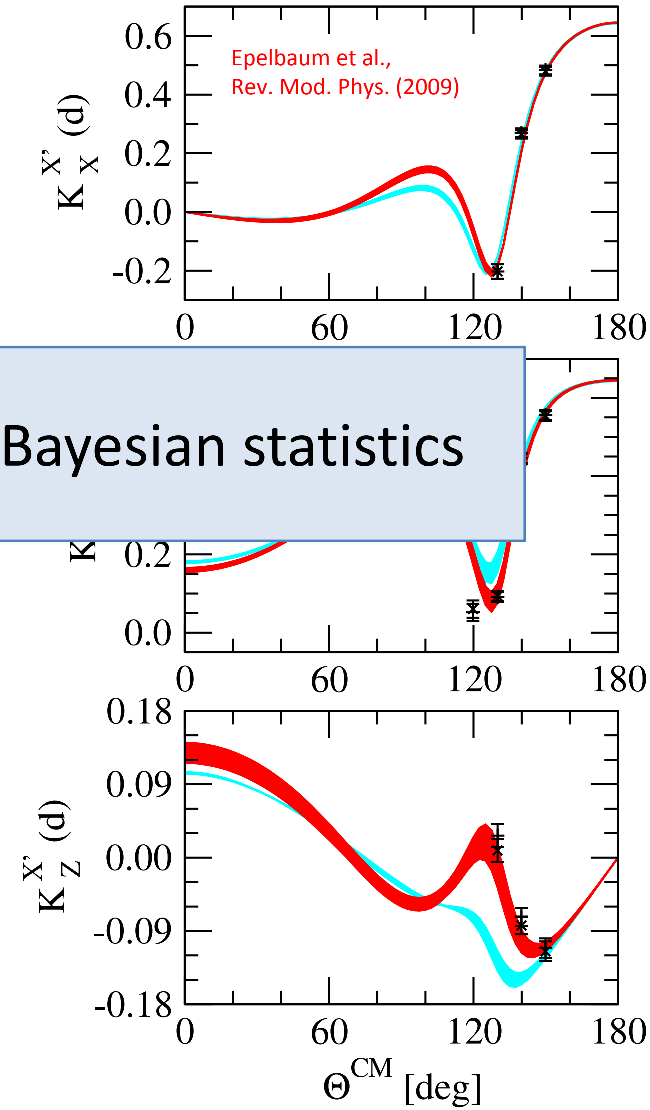

Motivated by naturalness to apply Bayesian statistics

Problems with this as UQ (see right figure):

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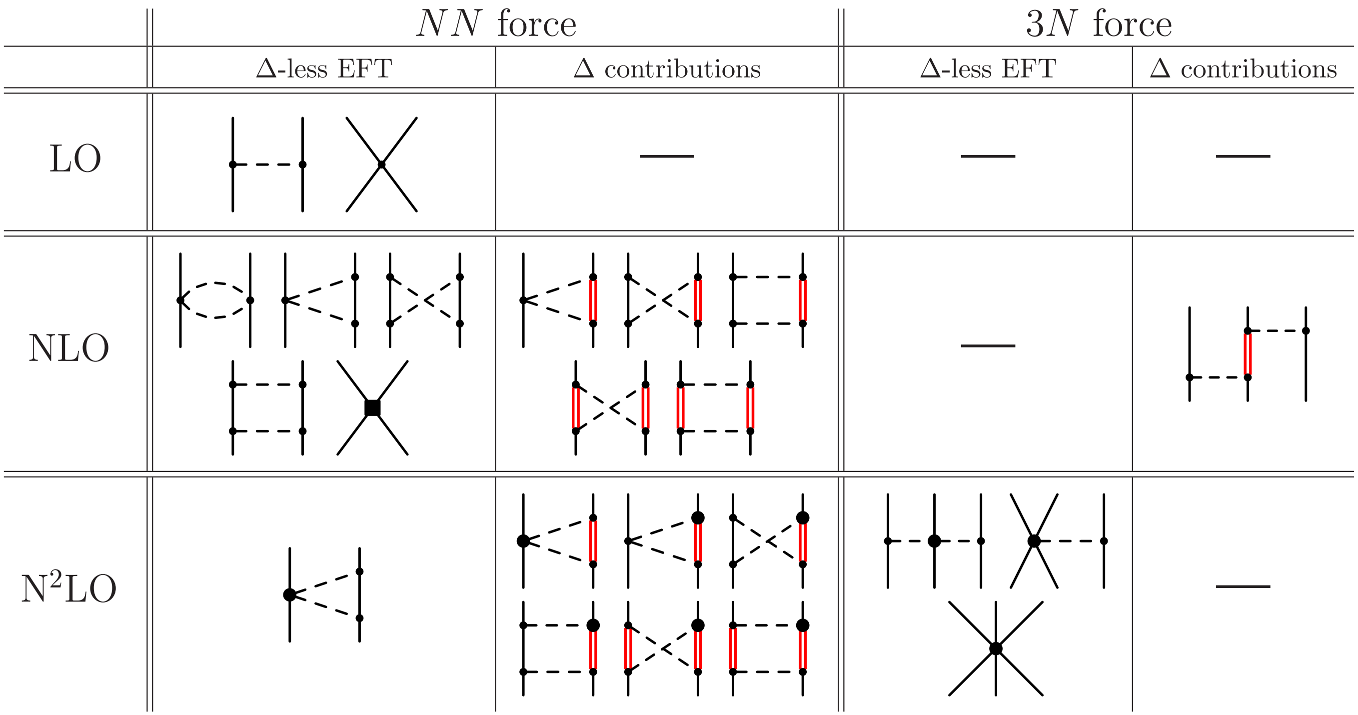
- often underestimates uncertainty
- statistical interpretation???
- Is the EFT actually working?

What kind of statistics problems do we have?



Having obtained a force, one needs to propagate uncertainties through *nonlinear* calculations (which are usually very expensive).

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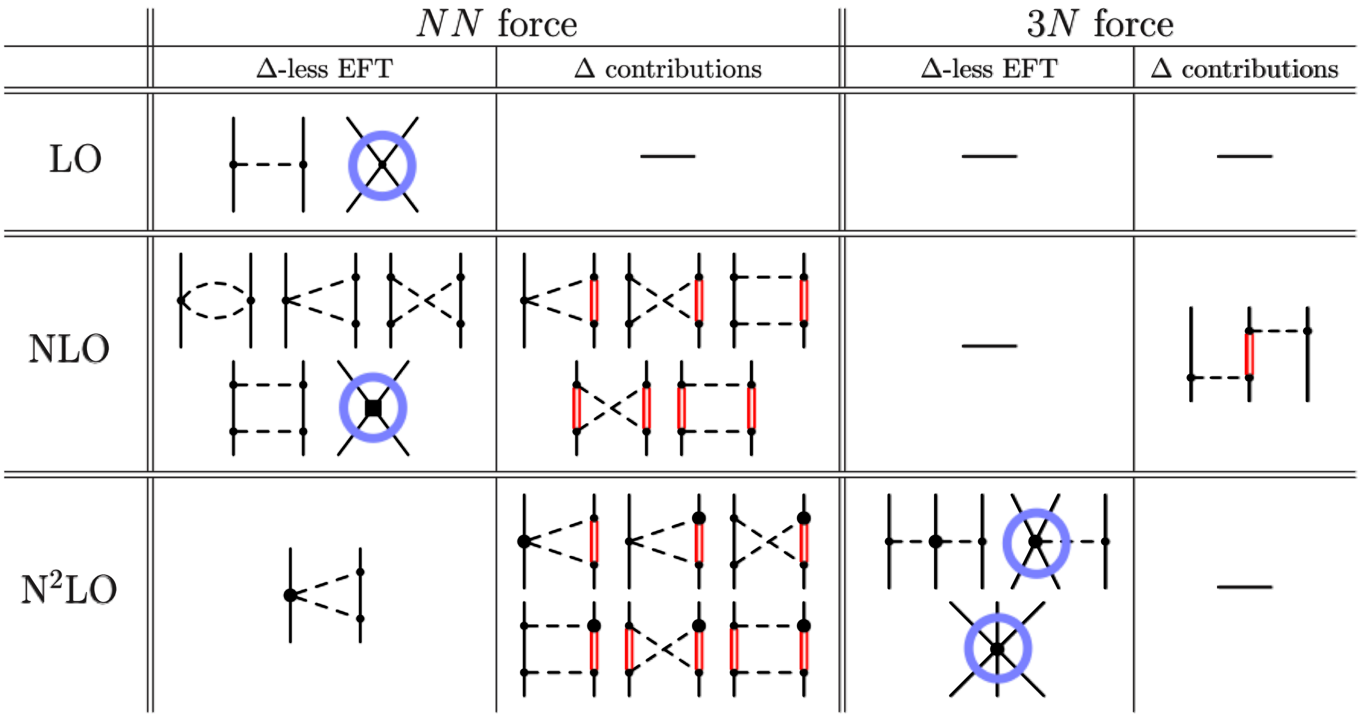
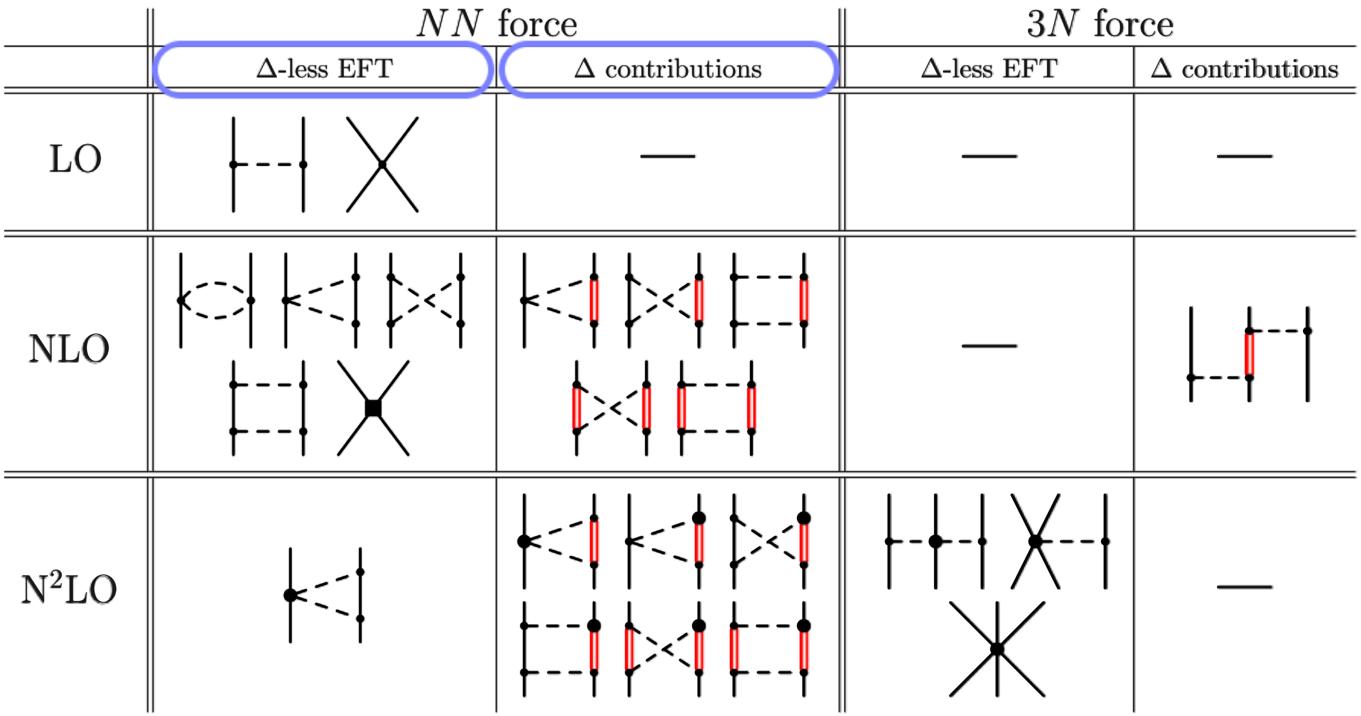


Parameter estimation (inverse problem)

Having obtained a force, one needs to propagate uncertainties through *nonlinear* calculations (which are usually very expensive).

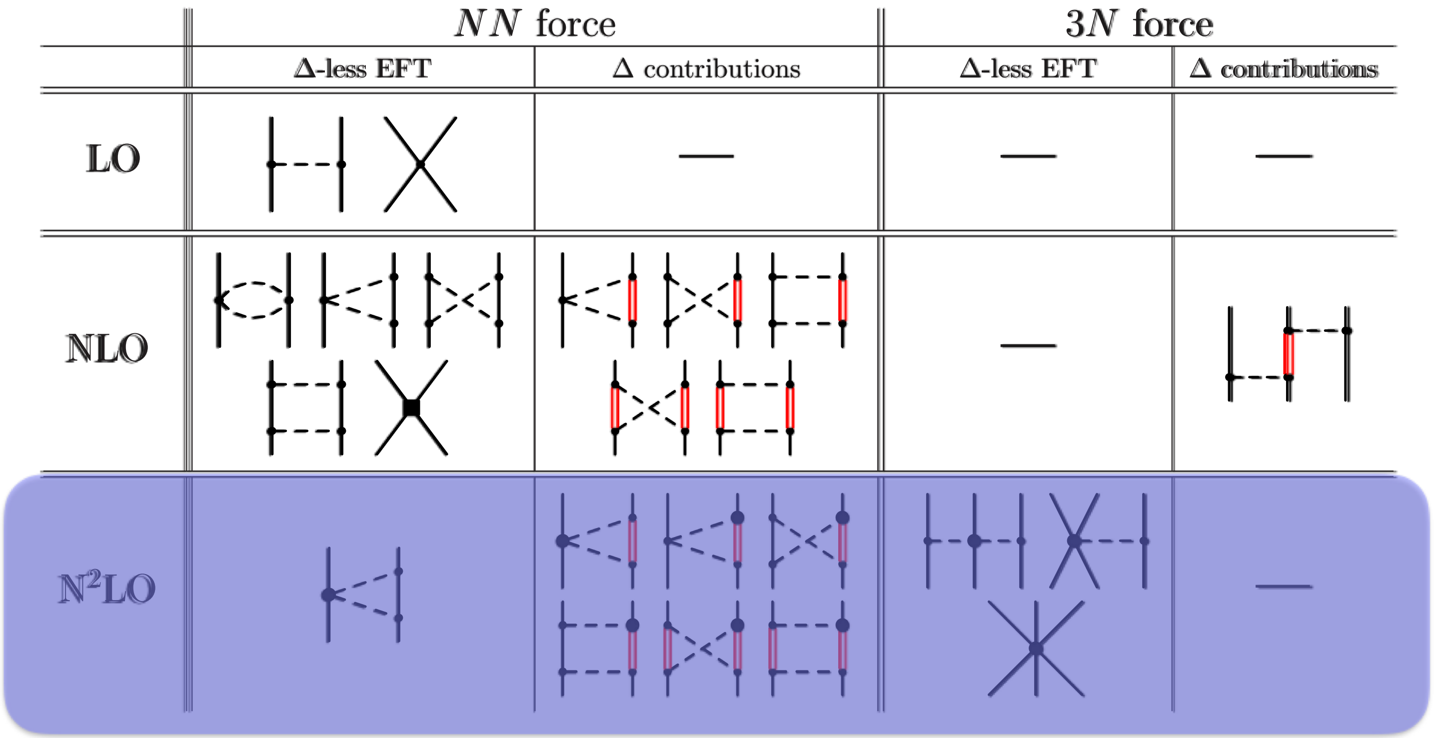
What kind of statistics problems do we have?



“Bayesian model selection”: What are the best degrees of freedom?

Having obtained a force, one needs to propagate uncertainties through *nonlinear* calculations (which are usually very expensive).

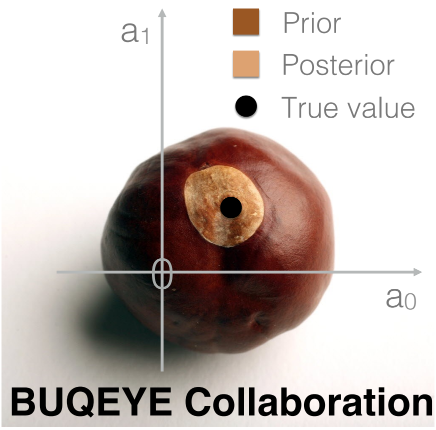
What kind of statistics problems do we have?



Truncation error (discrepancy): omitted higher-order diagrams

Having obtained a force, one needs to propagate uncertainties through *nonlinear* calculations (which are usually very expensive).

Bayesian Uncertainty Quantification: Errors for Your EFT



Overall goal:
Full uncertainty quantification (UQ) and associated diagnostics for EFT predictions using Bayesian statistics

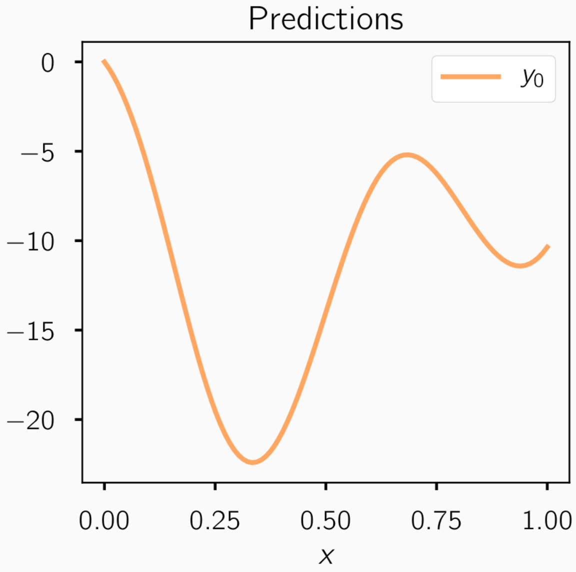
Dick Furnstahl (OSU)
Jordan Melendez (OSU)
Matt Pratola (OSU Statistics)
Harald Griesshammer (GWU)
Daniel Phillips (OU)
Sarah Wesolowski (SU)

- Experimentalists have long been careful practitioners of statistics, but theorists have not. In nuclear physics, the advent of precision calculations requires verifiable, robust theory UQ.
- Interaction with statisticians has been *invaluable*, including members of the SciDAC NUCLEI project and participants in workshops such as the 4-week INT program on “Bayesian Statistics in Nuclear Physics”, e.g., Derek Bingham, Dave Higdon (INT co-organizer), Earl Lawrence, Ian Vernon, Frederi Viens, …
- A particularly exciting spin-off is we have found physics *discovery* with statistics!

Representing an EFT expansion: Toy model example

- Theoretical predictions could look like the following

$\{y_0\}$



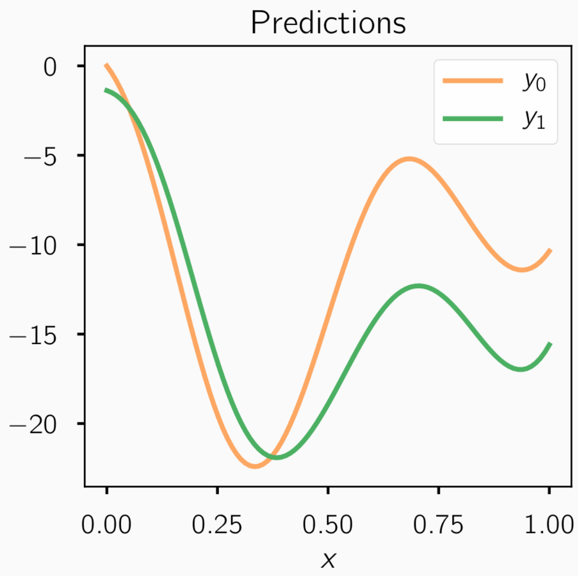
$y_0 \to \mathrm{LO}$

- The y_i are predictions depending on x (could be energy, scattering angle, …)

Representing an EFT expansion: Toy model example

- Theoretical predictions could look like the following

$$\{y_0, y_1\}$$



$$y_0 \longrightarrow \text{LO}$$

$$y_1 \longrightarrow \text{NLO}$$

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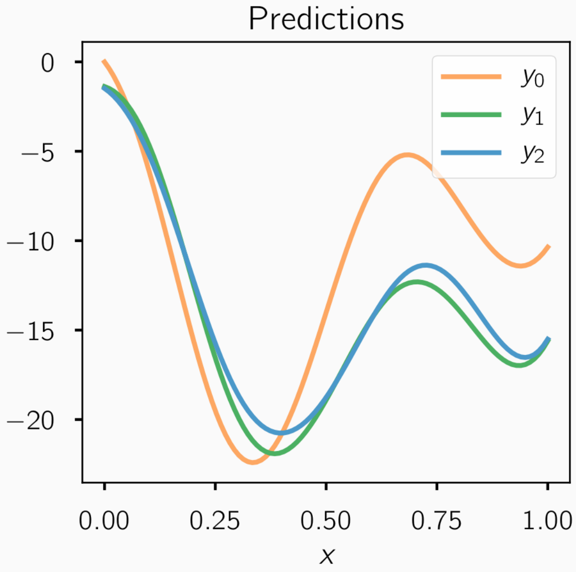
Representing an EFT expansion: Toy model example

- Theoretical predictions could look like the following

$$\{y_0, y_1, y_2\}$$



$y_0 \to \mathrm{LO}$

$y_1 \to \mathrm{NLO}$

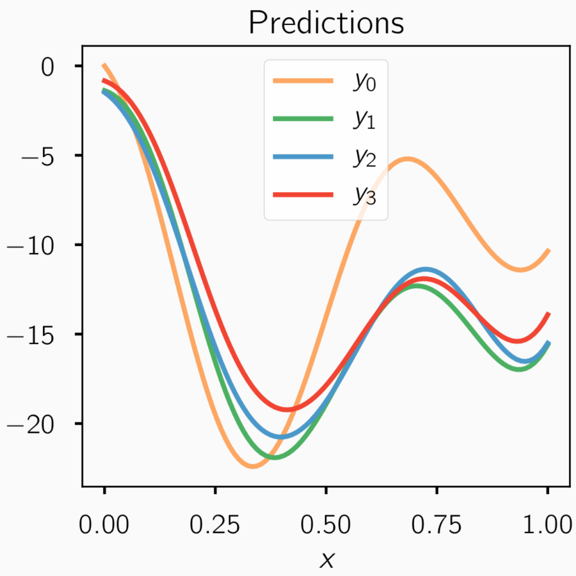
$y_2 \to \mathrm{N^2LO}$

- The y_i are predictions depending on x (could be energy, scattering angle, …)

Representing an EFT expansion: Toy model example

- Theoretical predictions could look like the following

$$\{y_0, y_1, y_2, y_3\}$$



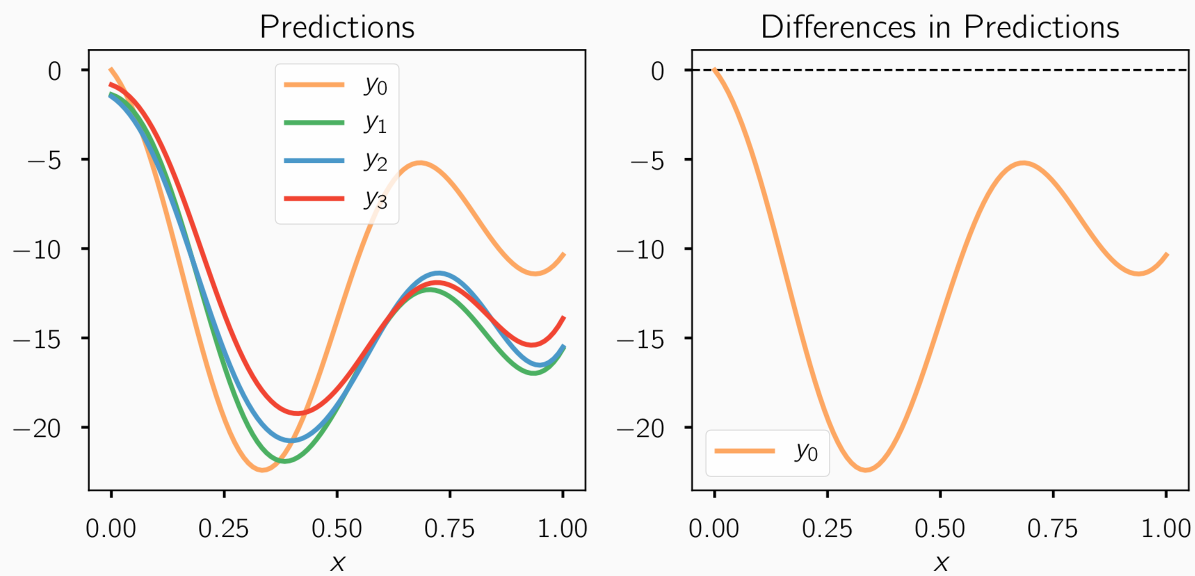
$$y_0 \rightarrow \mathrm{LO}$$
$$y_1 \rightarrow \mathrm{NLO}$$
$$y_2 \rightarrow \mathrm{N^2LO}$$
$$\vdots$$
$$y_k \rightarrow \mathrm{N^kLO}$$

- The y_i are predictions depending on x (could be energy, scattering angle, …)

Representing an EFT expansion: Toy model example

- Theoretical predictions could look like the following
- One can change variables for convenience/insight.

$$y_0 = y_0$$



- The y_i are predictions depending on x (could be energy, scattering angle, …)
- y_{ref} is are reference scale, Q is a dimensionless expansion parameter

$$\text{c.f. } K(v^2) \approx \underbrace{(mv^2/2)}_{y_{\text{ref}}}[b_0 + b_2 \underbrace{(v/c)^2}_{Q^2} + b_4(v/c)^4 + \mathcal{O}(1)(v/c)^4 + \cdots]$$

Representing an EFT expansion: Toy model example

- Theoretical predictions could look like the following
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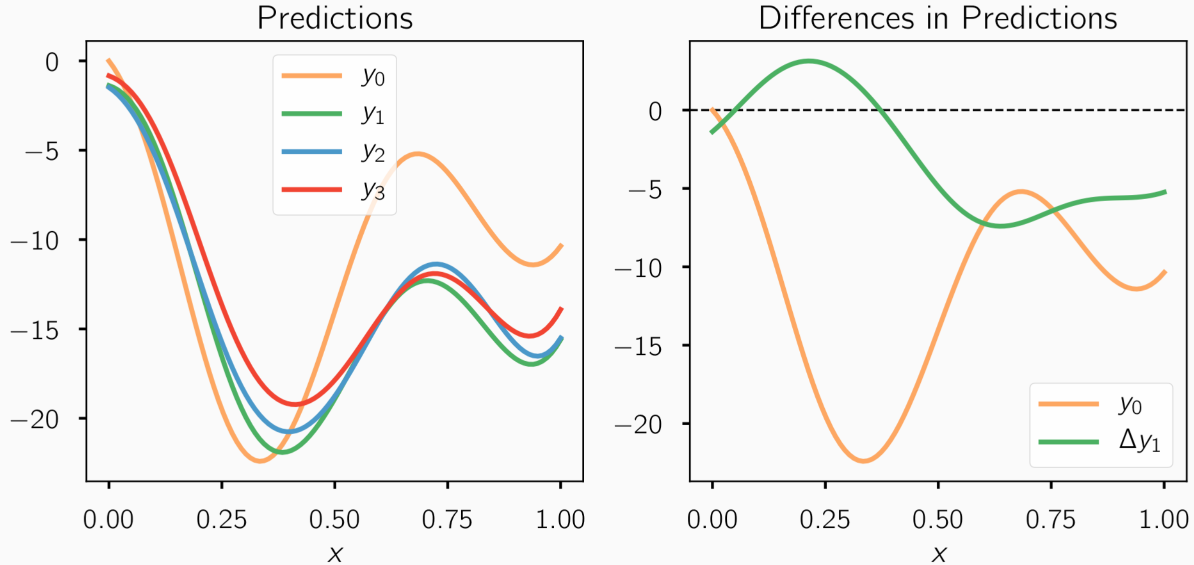
$$y_1 = y_0 + \Delta y_1$$



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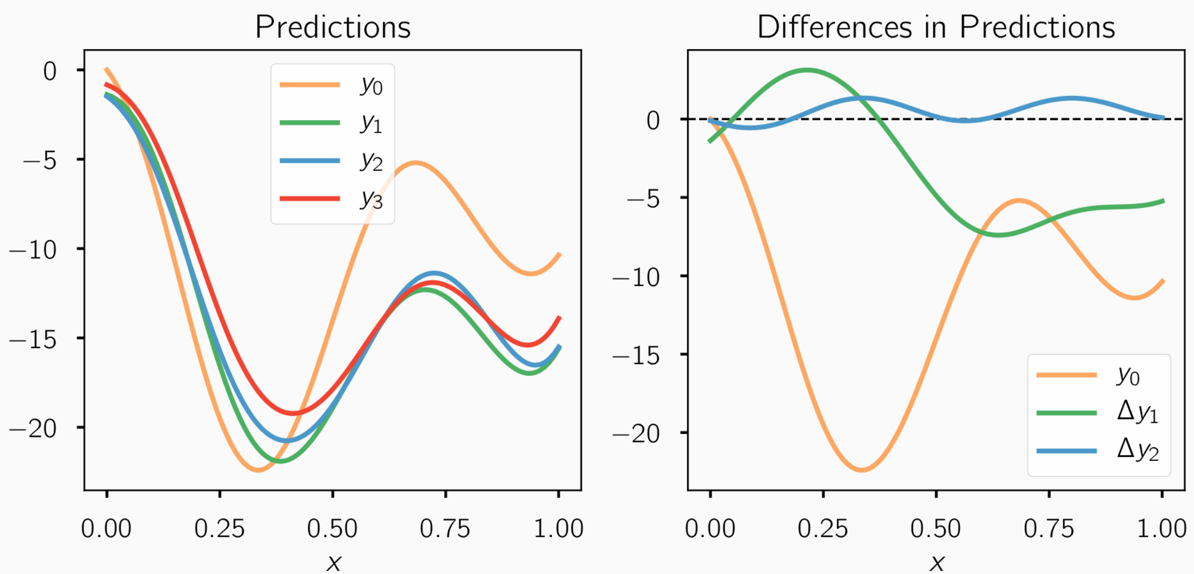
$$y_2 = y_0 + \Delta y_1 + \Delta y_2$$



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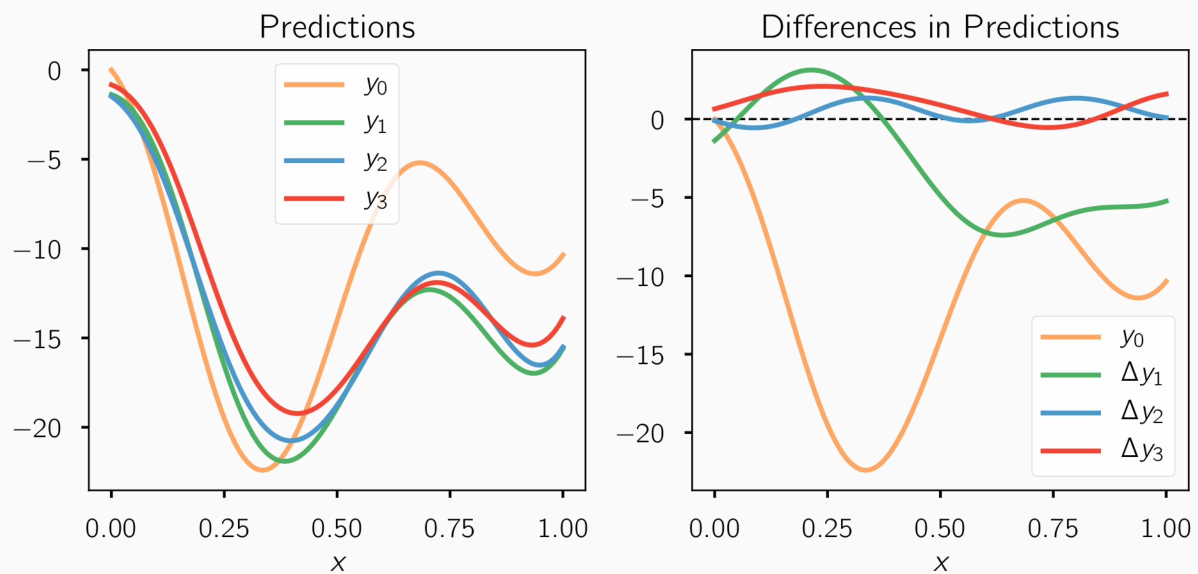
Representing an EFT expansion: Toy model example

- Theoretical predictions could look like the following
- One can change variables for convenience/insight.
- $\Delta y_n = y_{\text{ref}} c_n Q^n$

$$y_3 = y_0 + \Delta y_1 + \Delta y_2 + \Delta y_3$$



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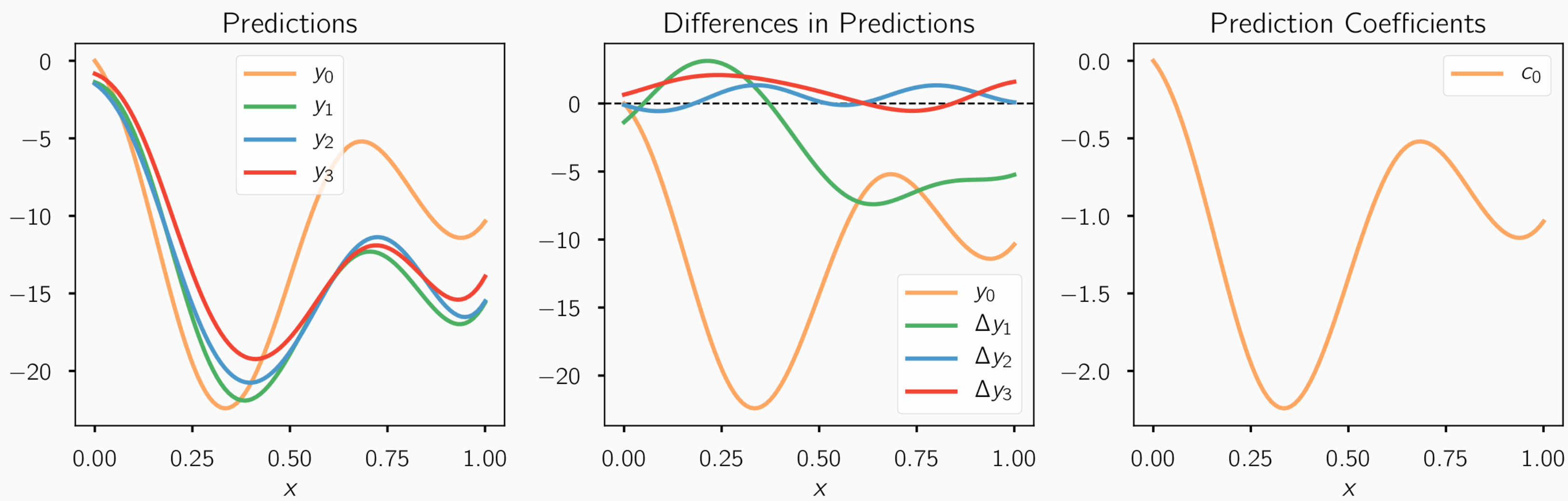

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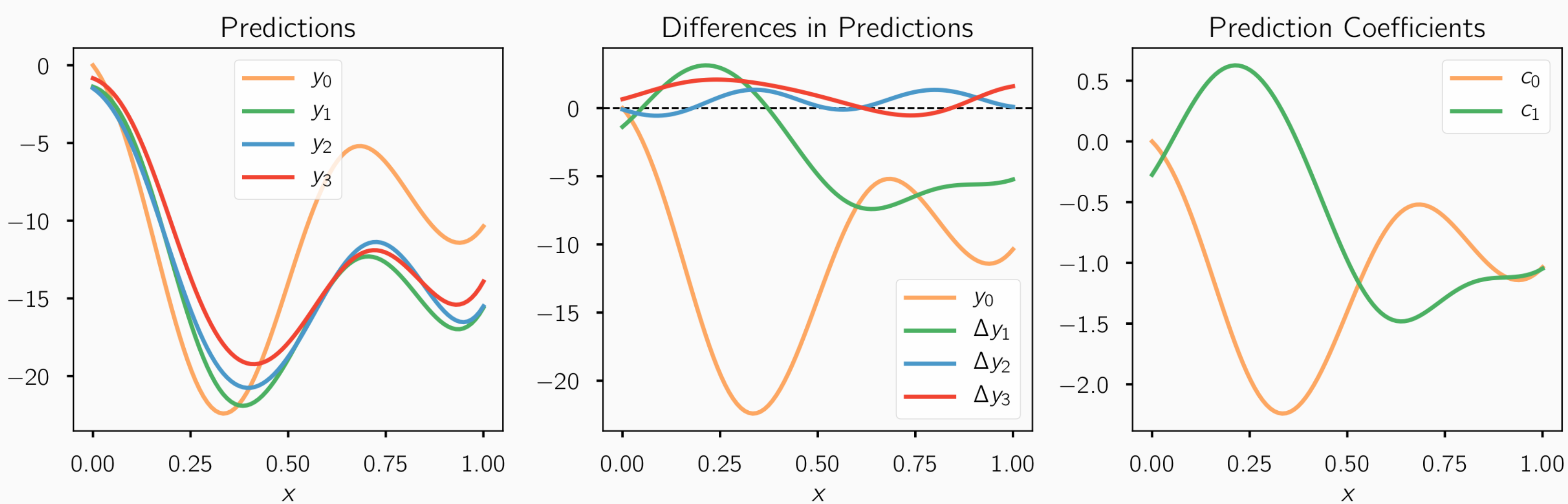

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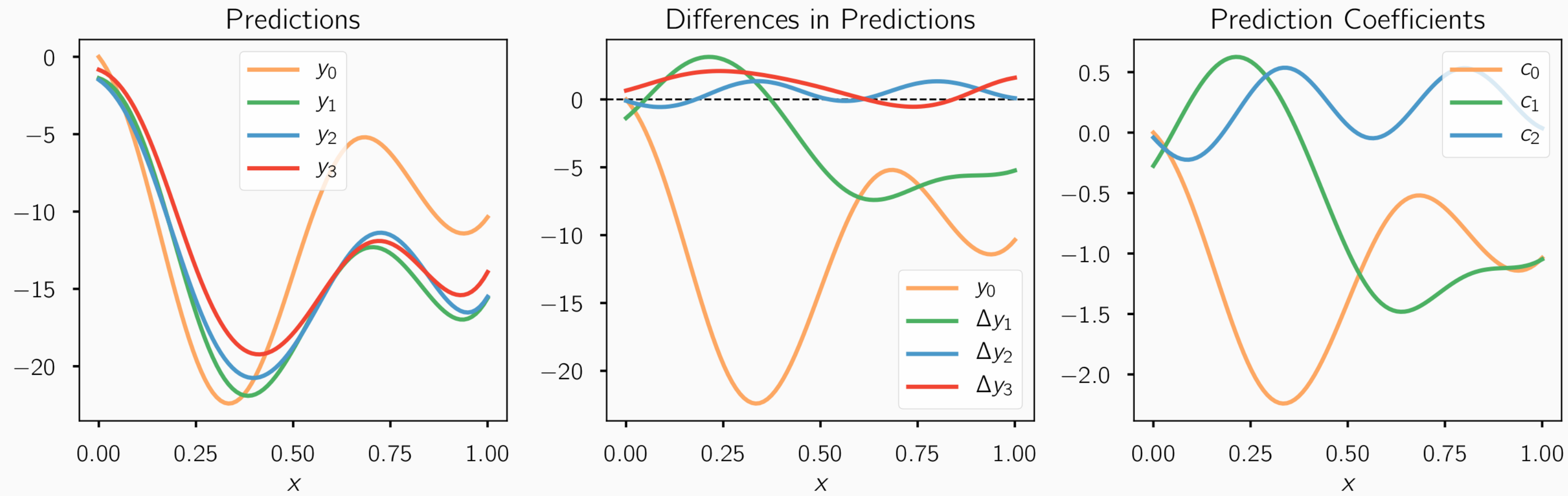

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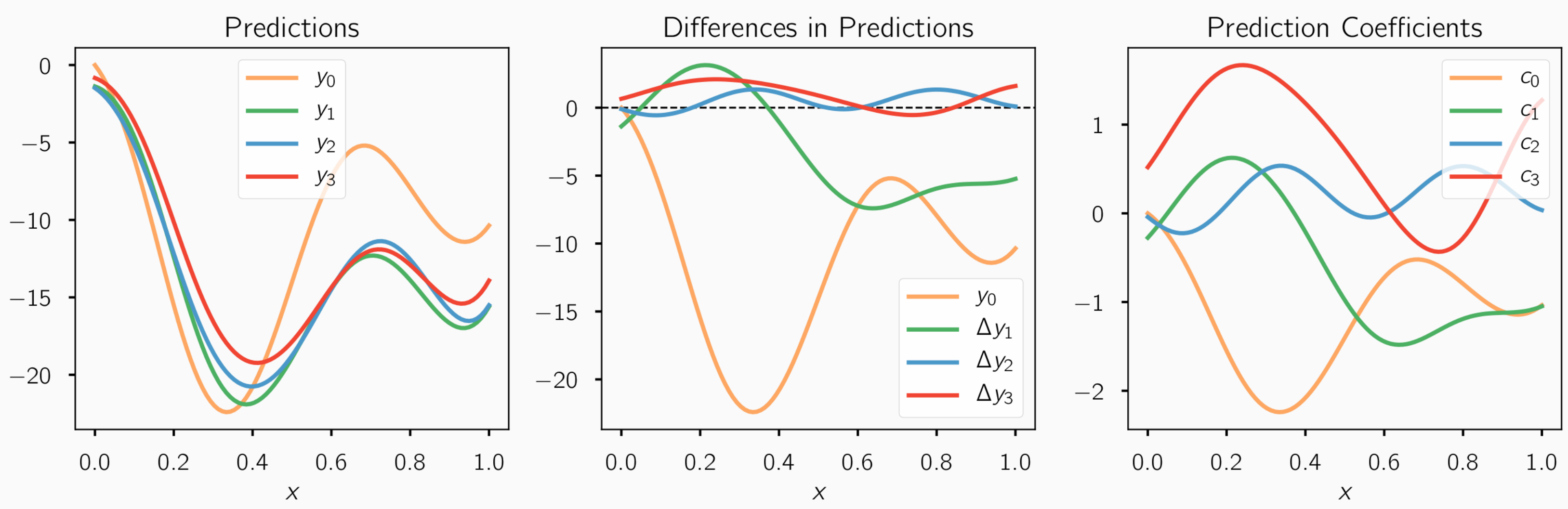

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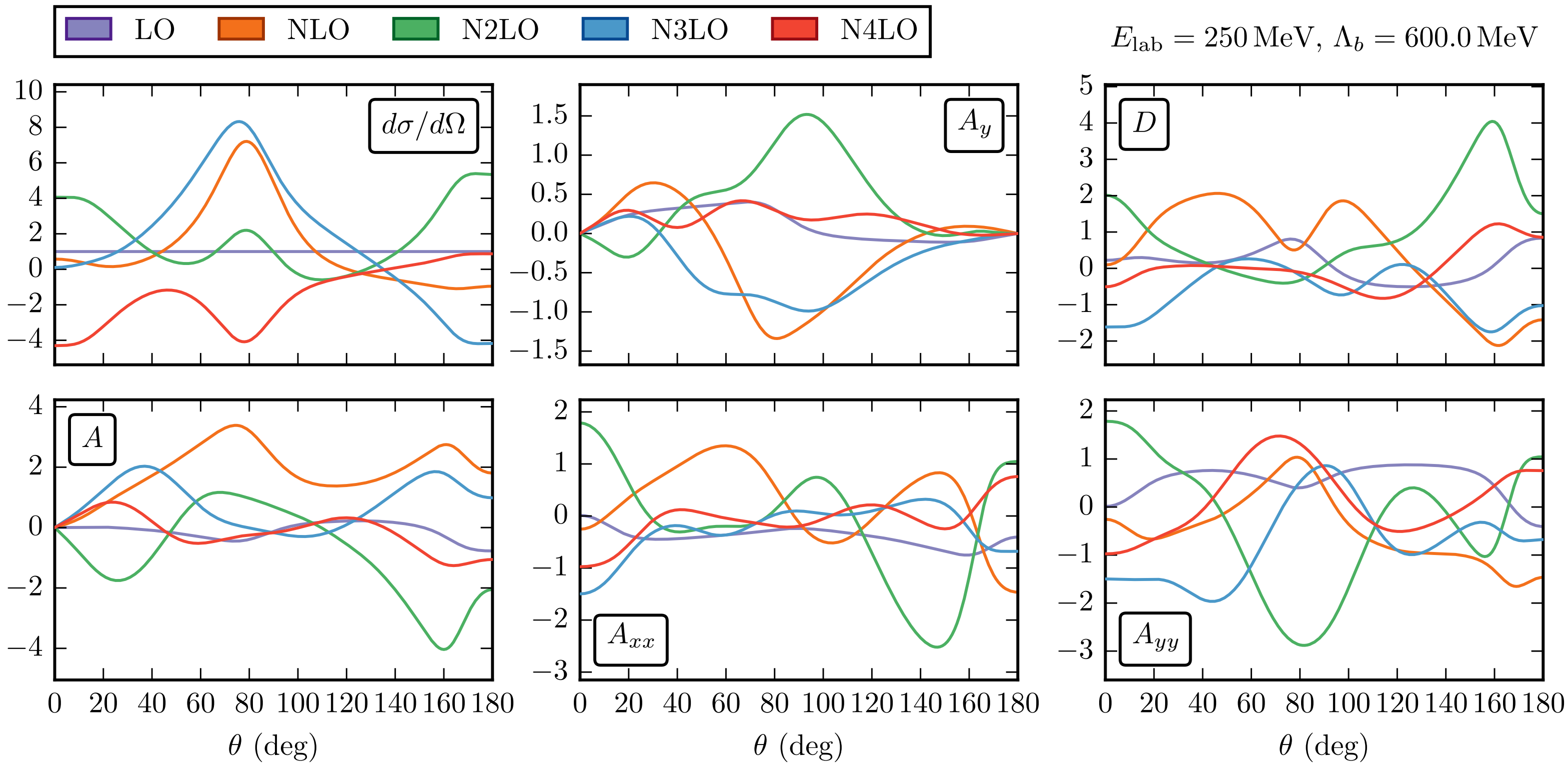
Does the toy model example look like the real world?

Use EKM semi-local interactions applied to NN scattering as example.

Eur. Phys. J. A 51, 53 (2015) and Phys. Rev. Lett. 115, 122301 (2015)

Angular observables overall: as a function of angle at single energy



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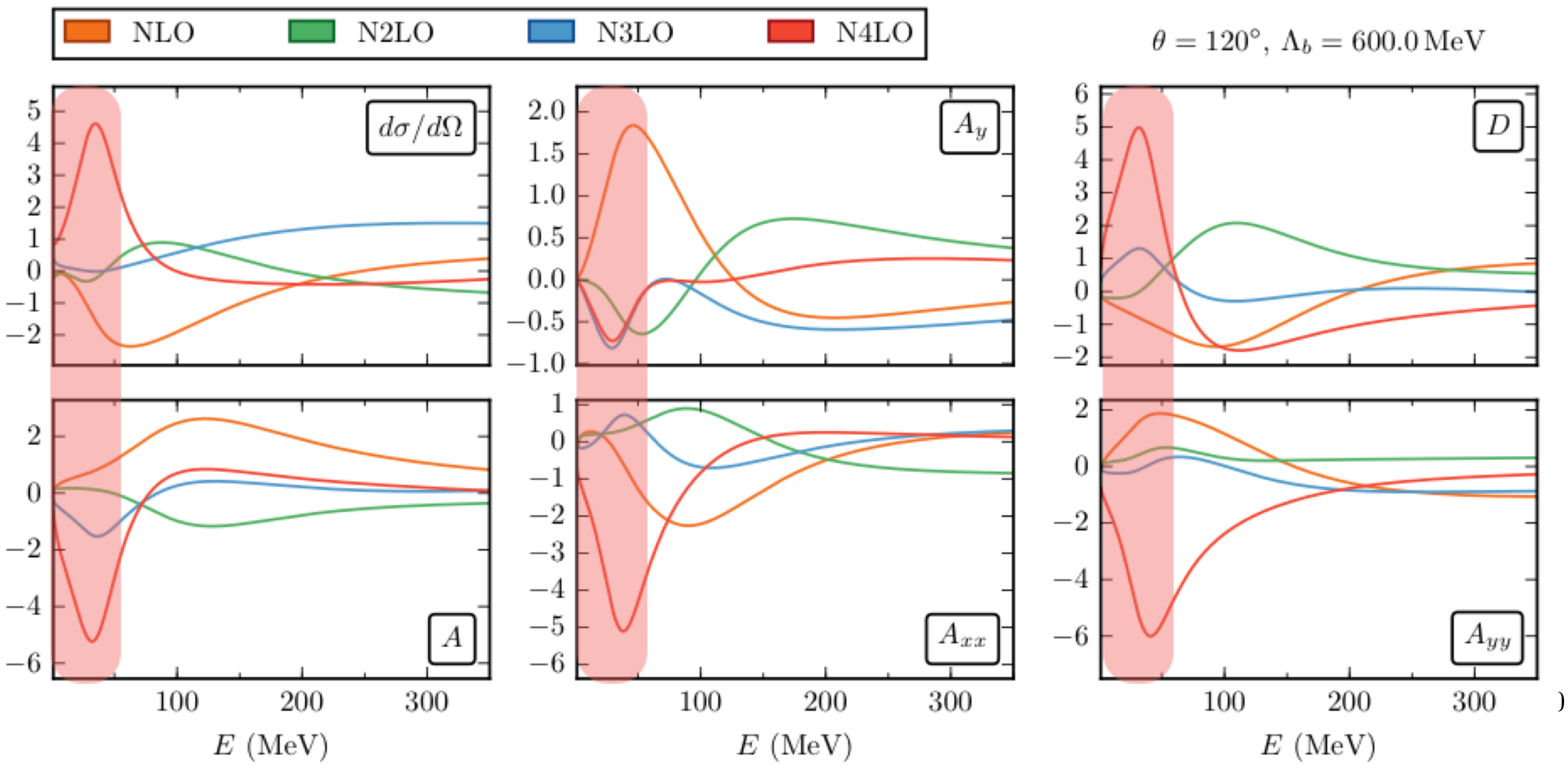
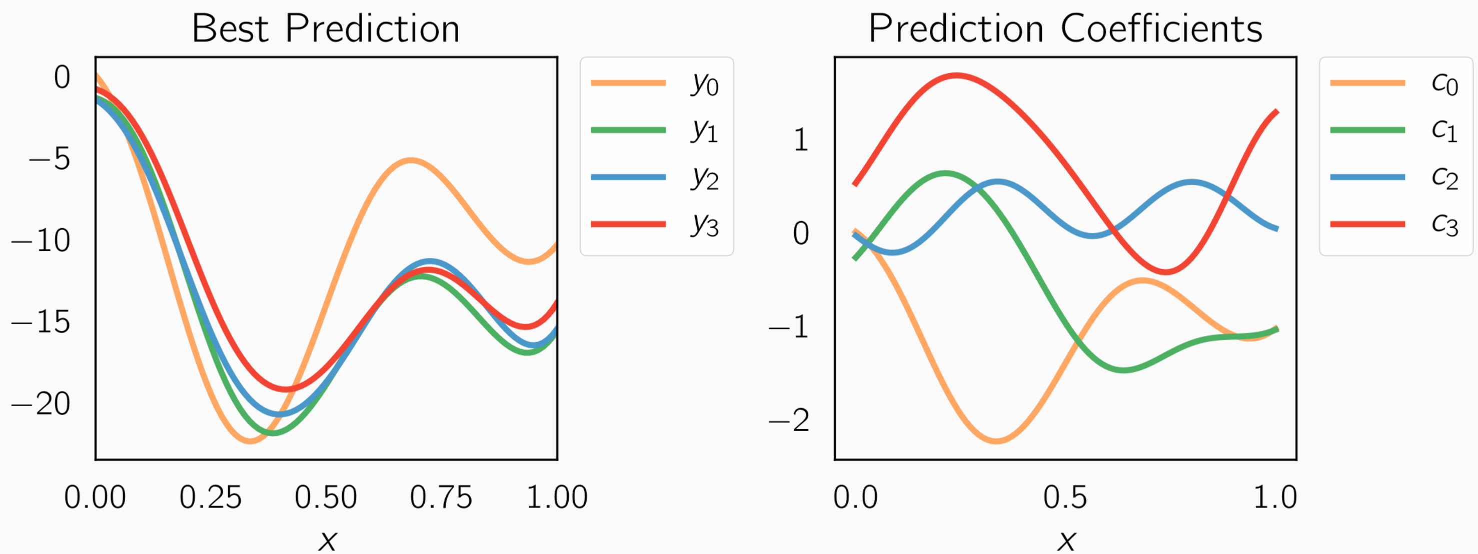


Representing an EFT expansion: Toy model example

Main equation

$$y_k = y_{\mathrm{ref}} \sum_{n=0}^{k} c_n Q^n$$

$$c_n \equiv \frac{y_n - y_{n-1}}{y_{\mathrm{ref}} Q^n}$$



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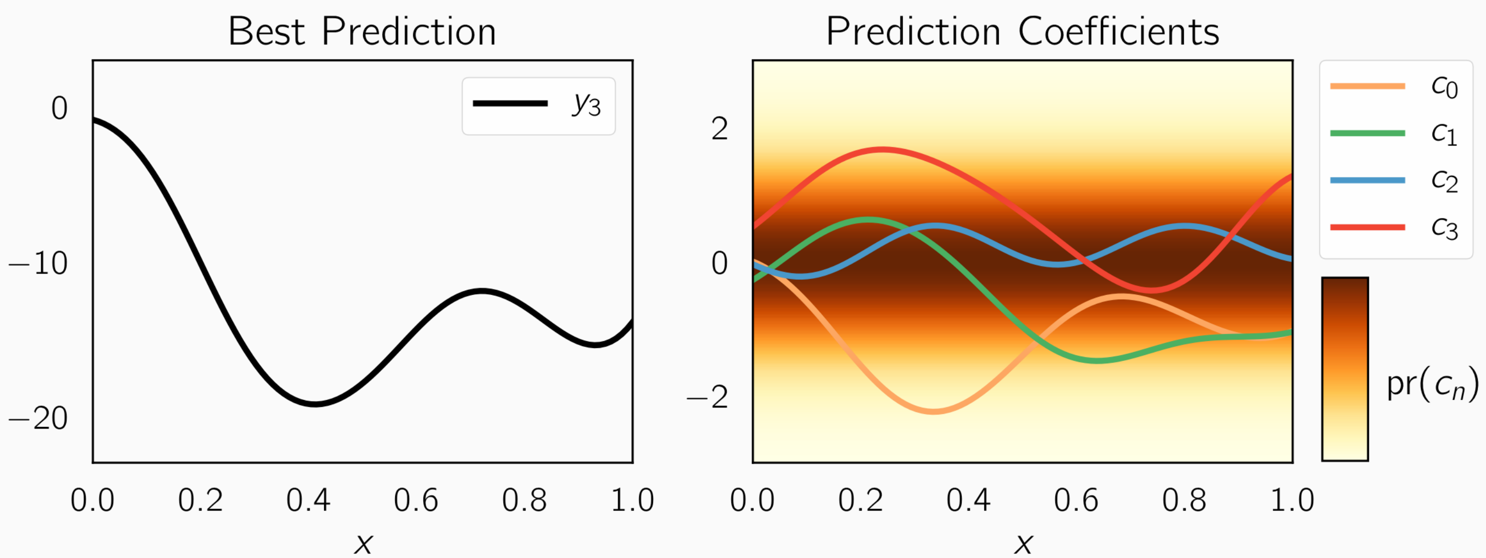
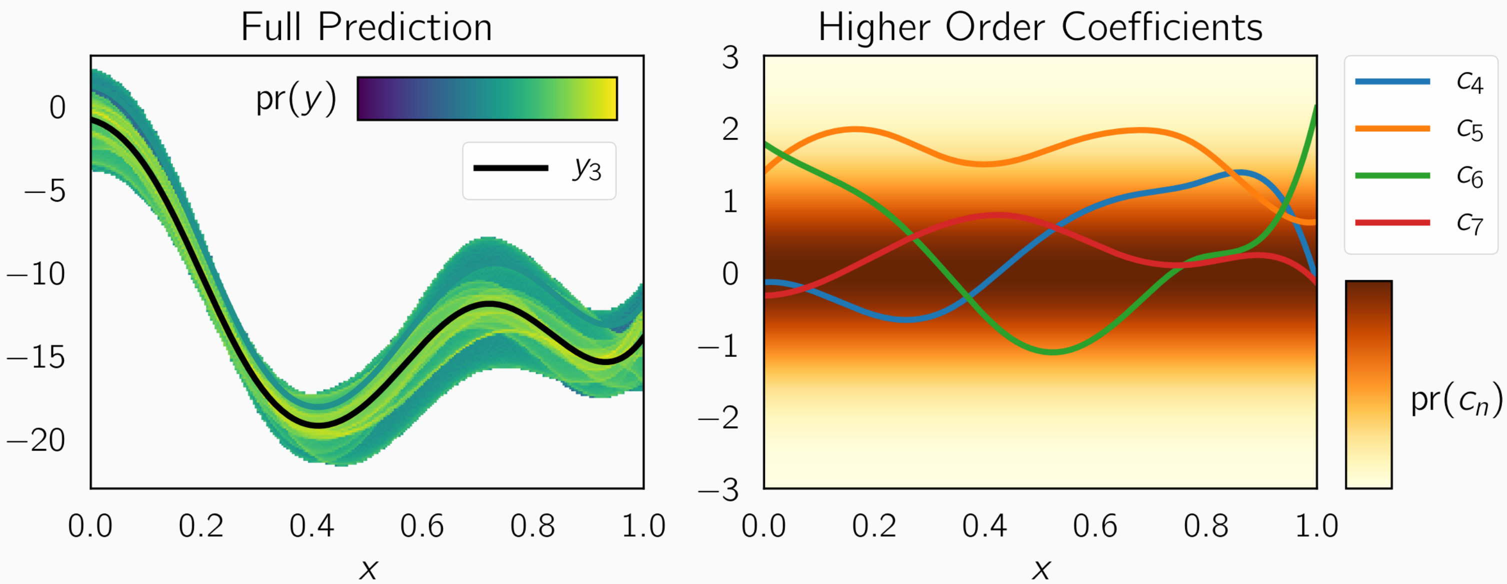


Representing an EFT expansion: Toy model example

Main equation

$$y = y_{\mathrm{ref}} \sum_{n=0}^{\infty} c_n Q^n$$

$$c_n \equiv \frac{y_n - y_{n-1}}{y_{\mathrm{ref}} Q^n}$$



- Can we derive $\mathrm{pr}(y|\{y_0, \cdots, y_k\}, Q, y_{\mathrm{ref}})$?
- Can we extract a posterior for the expansion parameter Q?

Hierarchial statistical model

- Decompose prediction

$$\mathcal{X}_k = \mathcal{X}_0 + \sum_{n=1}^{k} \Delta\mathcal{X}_n$$

[Note: here X_i are the observables instead of y_i.]

Hierarchial statistical model

- Decompose prediction

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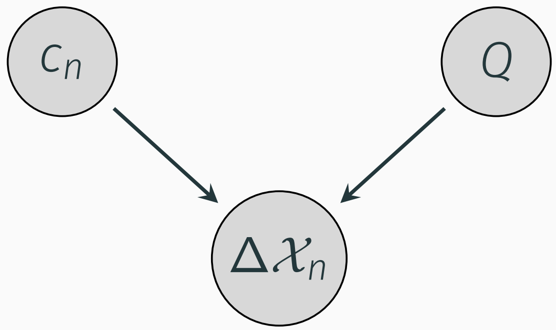
$$= \mathcal{X}_{\mathrm{ref}} \sum_{n=0}^{k} c_n Q^n$$

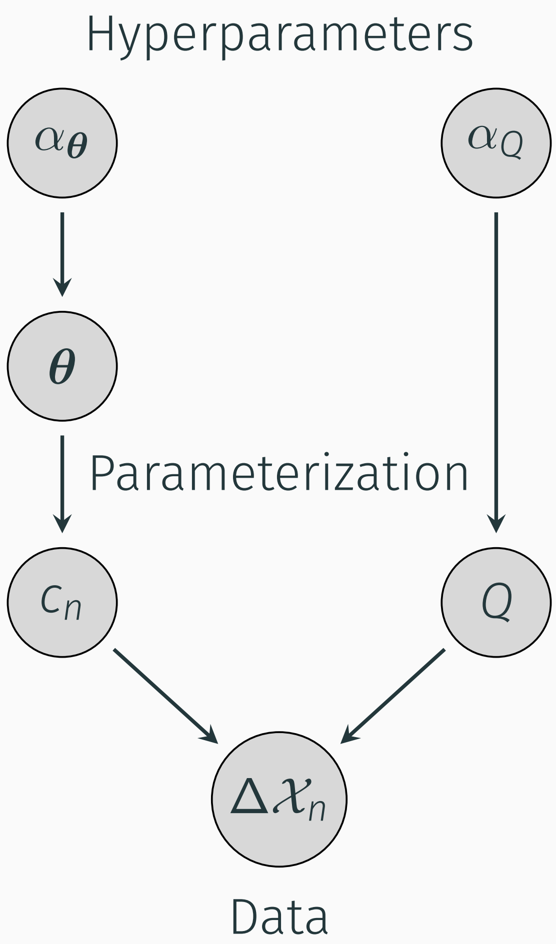
Parameterization



Data

[Note: here X_i are the observables instead of y_i.]

Hierarchial statistical model



- Decompose prediction

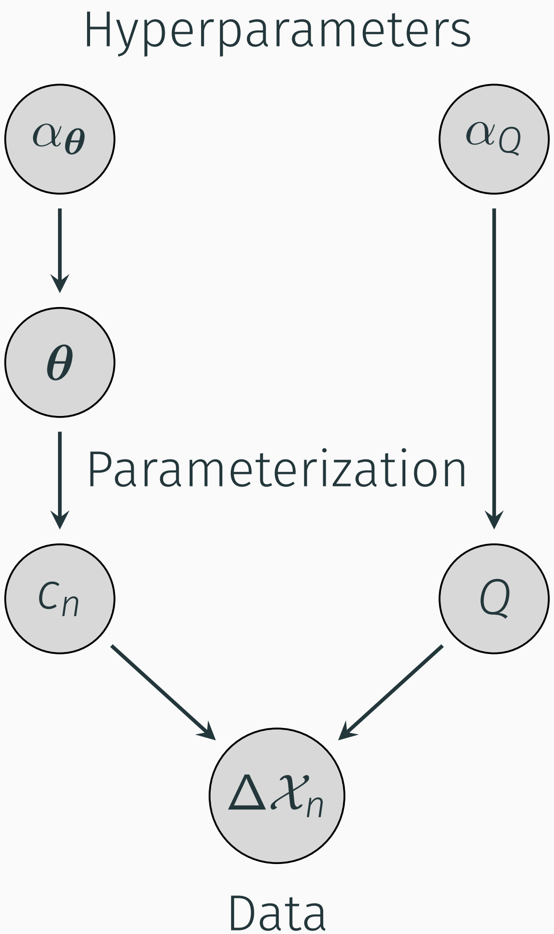
$$\mathcal{X}_k = \mathcal{X}_0 + \sum_{n=1}^{k} \Delta\mathcal{X}_n$$
$$= \mathcal{X}_{\text{ref}} \sum_{n=0}^{k} c_n Q^n$$

- Put priors on c_n (and Q)

$$c_n \mid \boldsymbol{\theta} \overset{\text{iid}}{\sim} \mathcal{GP}(\mu, \sigma^2 R_\ell)$$

[Note: here X_i are the observables instead of y_i.]

Hierarchial statistical model



- Decompose prediction

$$\mathcal{X}_k = \mathcal{X}_0 + \sum_{n=1}^{k} \Delta\mathcal{X}_n$$
$$= \mathcal{X}_{\text{ref}} \sum_{n=0}^{k} c_n Q^n$$

- Put priors on c_n (and Q)

$$c_n \mid \boldsymbol{\theta} \overset{\text{iid}}{\sim} \mathcal{GP}(\mu, \sigma^2 R_\ell)$$

- Learn $\boldsymbol{\theta}$ and Q

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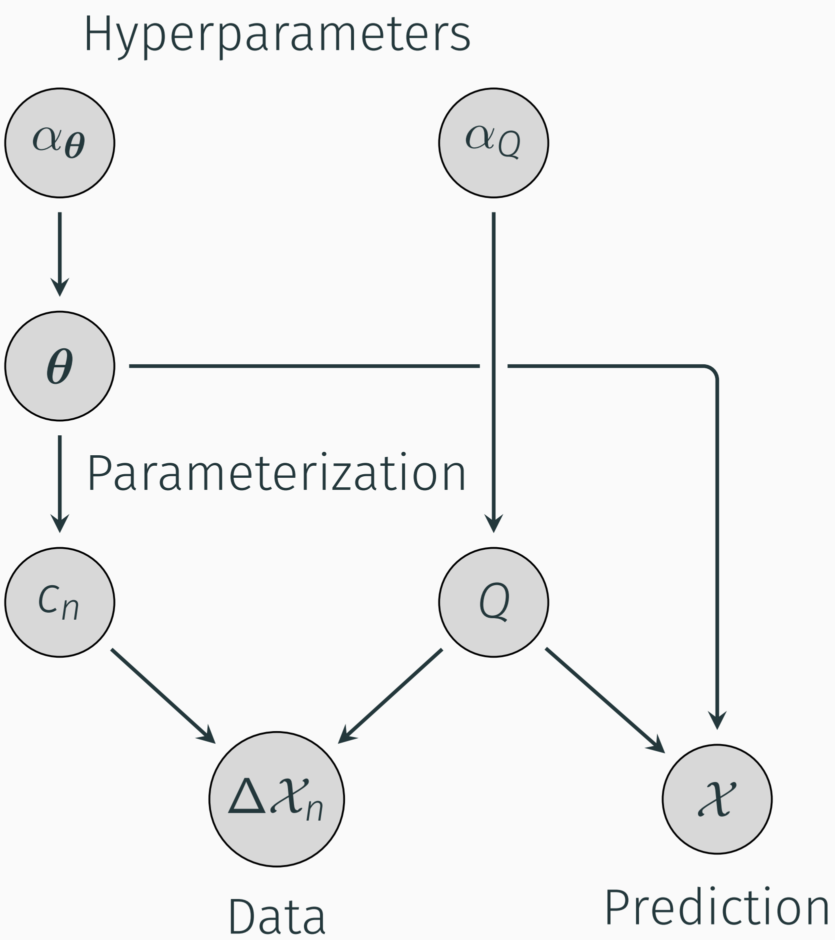

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- Learn $\boldsymbol{\theta}$ and Q
- Predict $\mathrm{pr}(\mathcal{X} \mid \mathcal{D})$

[Note: here X_i are the observables instead of y_i.]

Gaussian process priors

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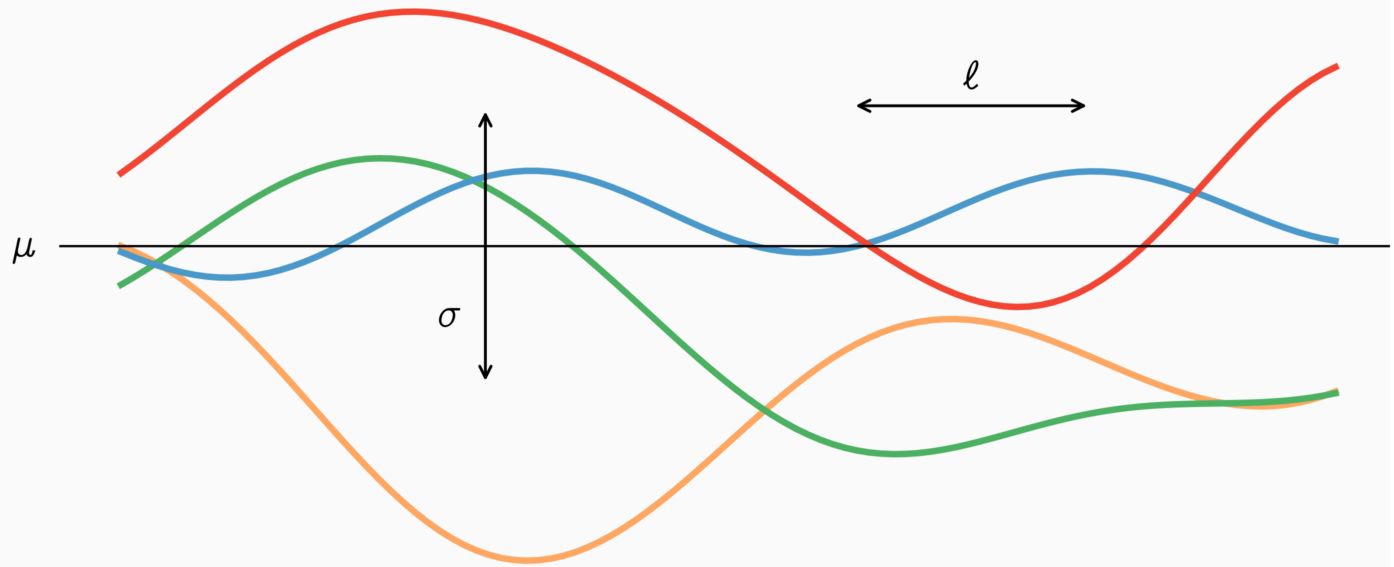

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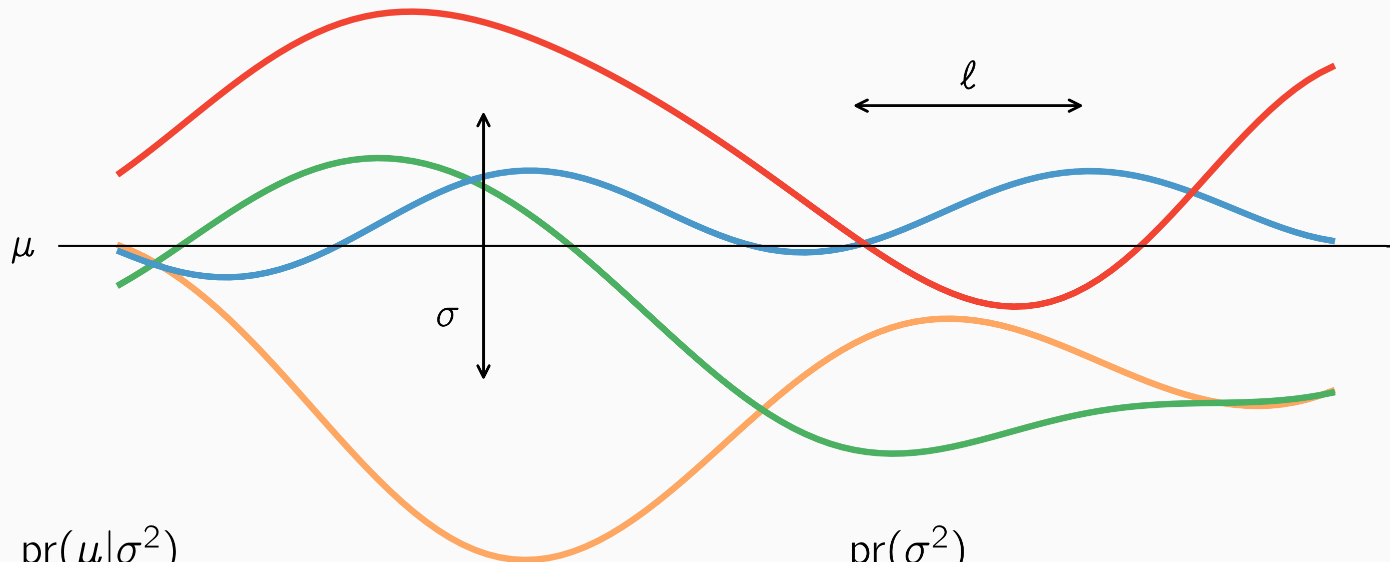
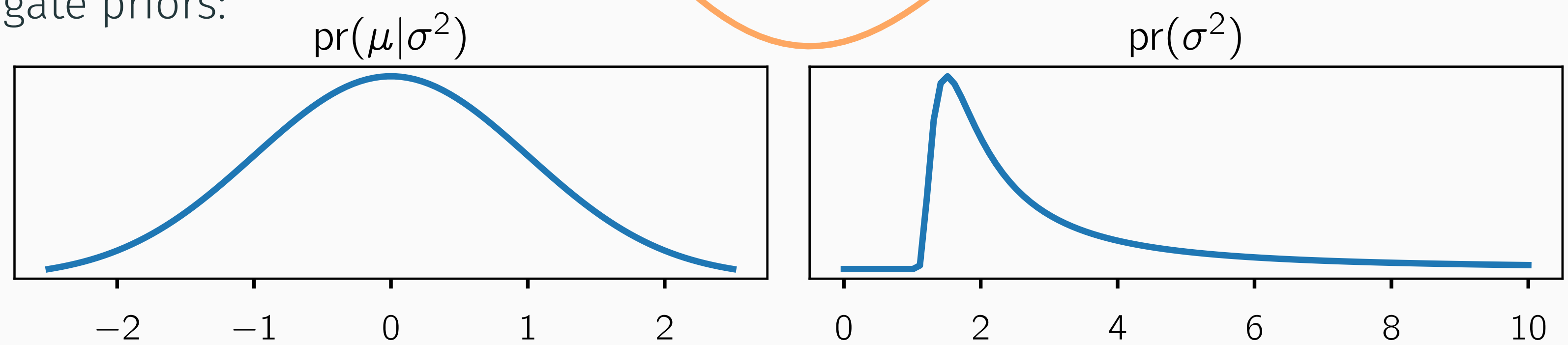
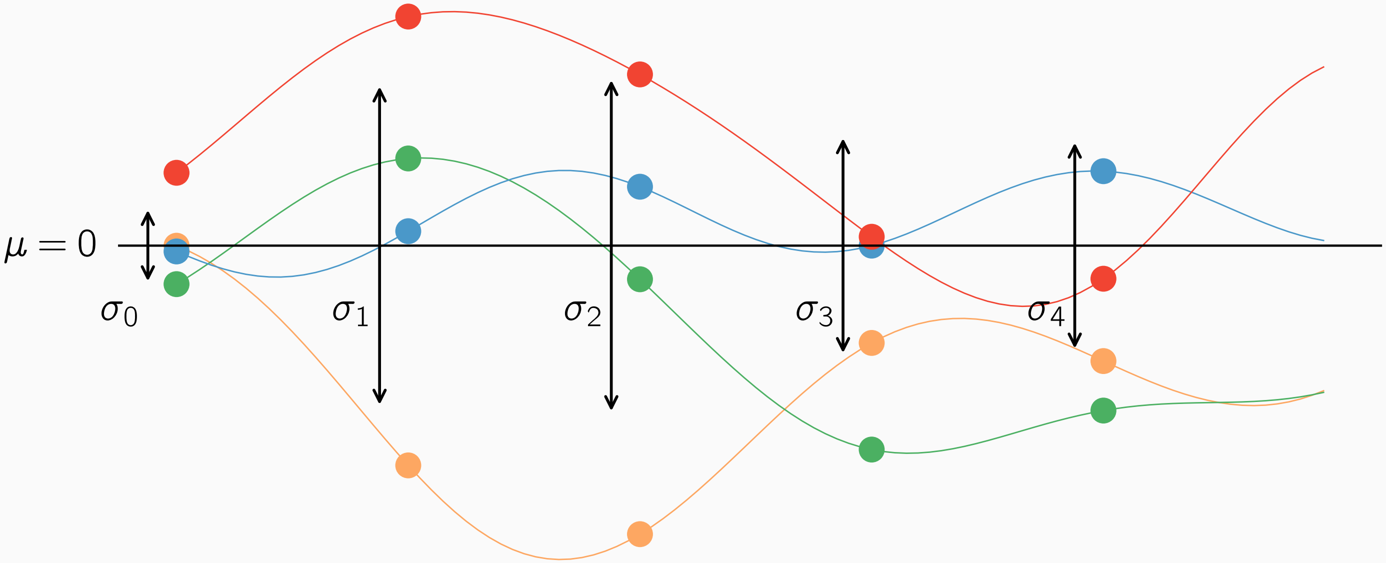


Conjugate priors:



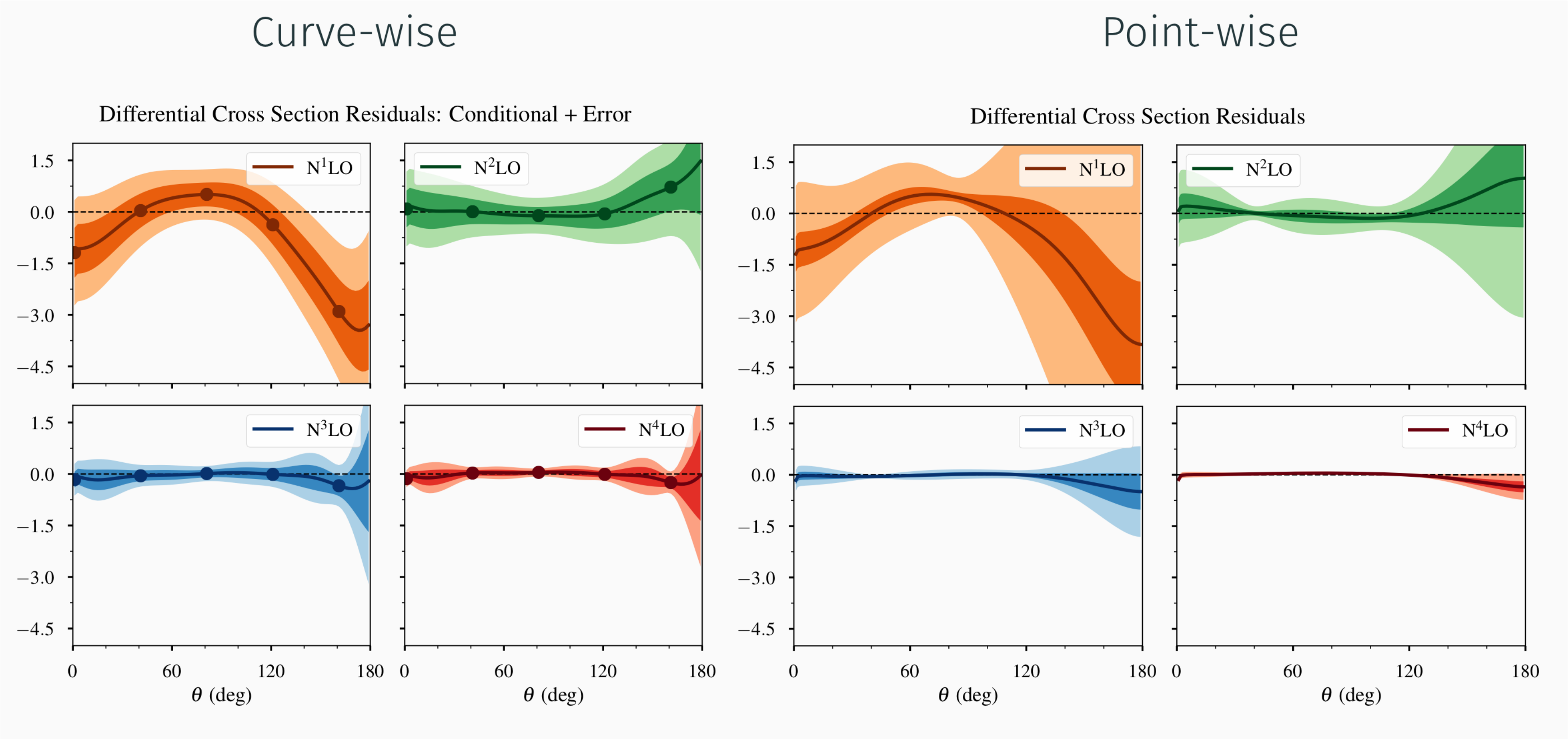
Gaussian process priors

$c_n \mid \sigma^2 \overset{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2)$



Contrast the Gaussian process model with our initial point-wise model.

Error bands for real-world calculations: EKM, R = 0.9 fm



Seems systematic and reasonable. How do we know it is working?

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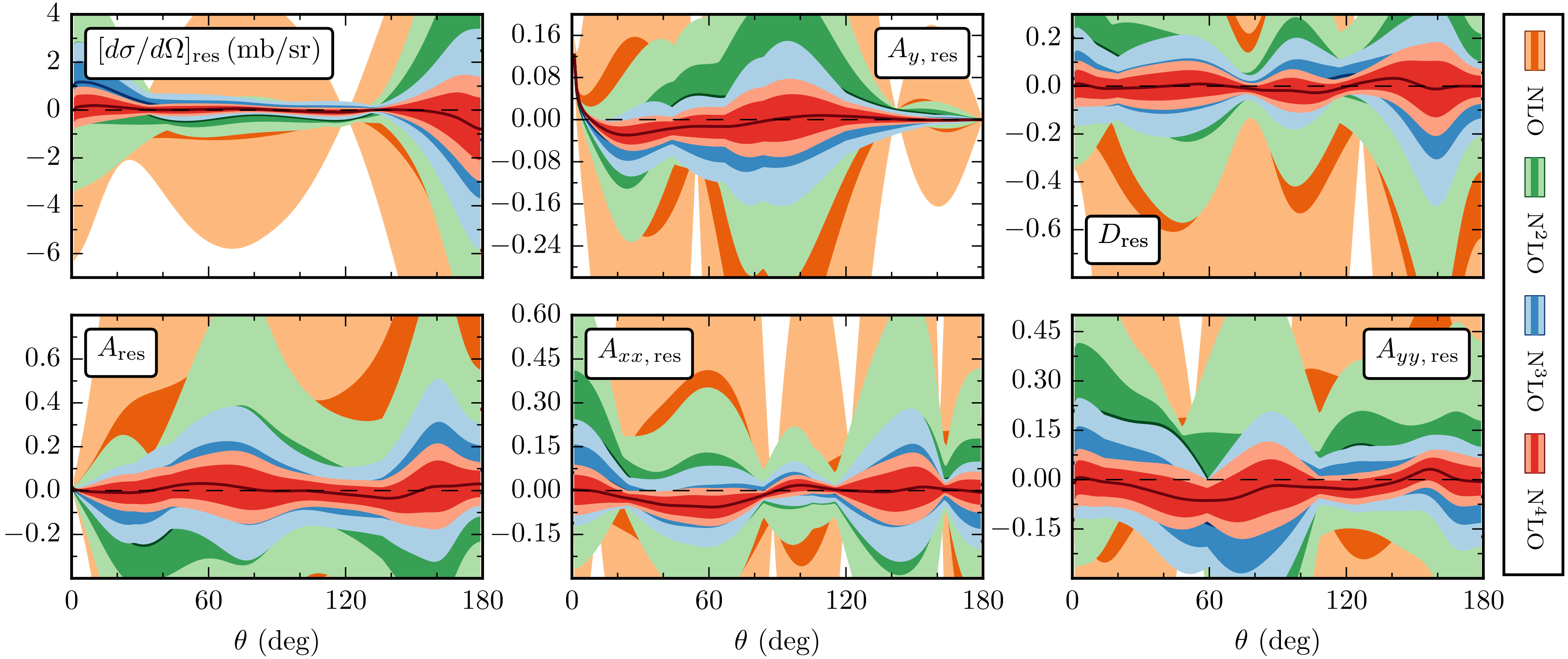

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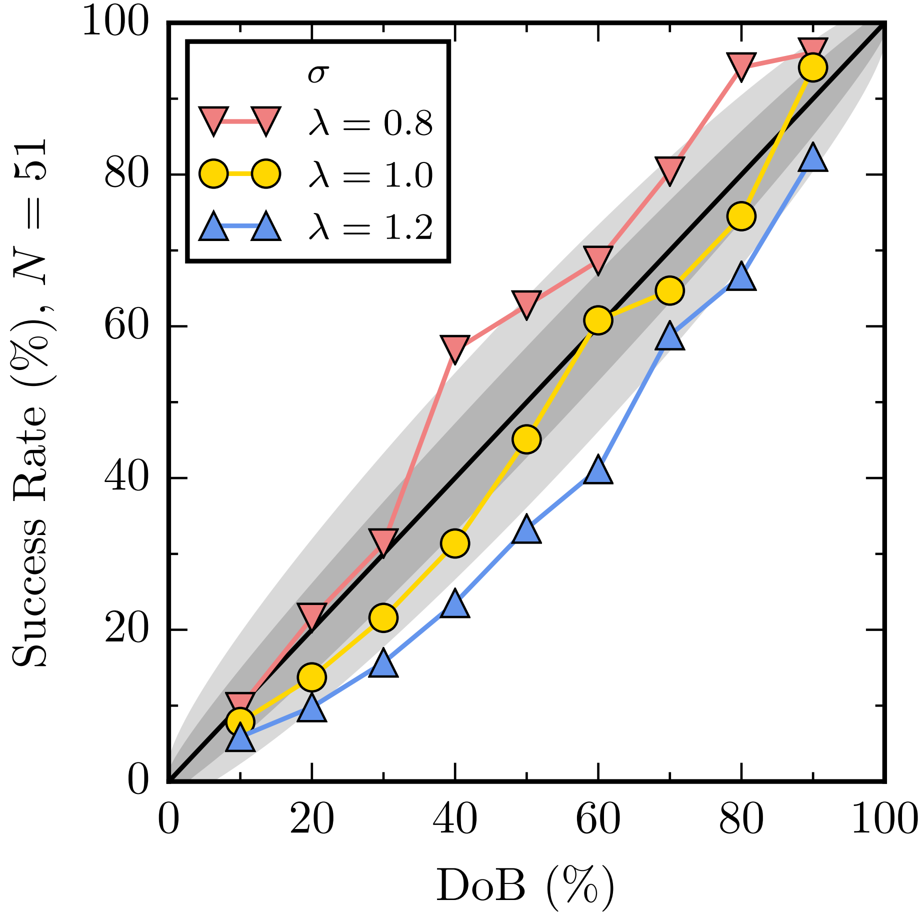
Model checking: Credible interval diagnostics

Melendez et al., PRC **96**, 024003 (2017)



$$X(p) = X_0 \sum_{n=0}^{k} c_n \lambda^n \left(\frac{p}{\lambda \times \Lambda_b} \right)^n$$

- Choose N predictions of observable (N=51)
- Here: total cross section at many energies
- How often does the (k+1)th prediction lie in the p% error band for prediction at kth order?

- Another check: vary expansion parameter
- $\lambda > 1$ indicates larger breakdown favored
- $\lambda < 1$ indicates smaller breakdown favored

Model checking: Credible interval diagnostics

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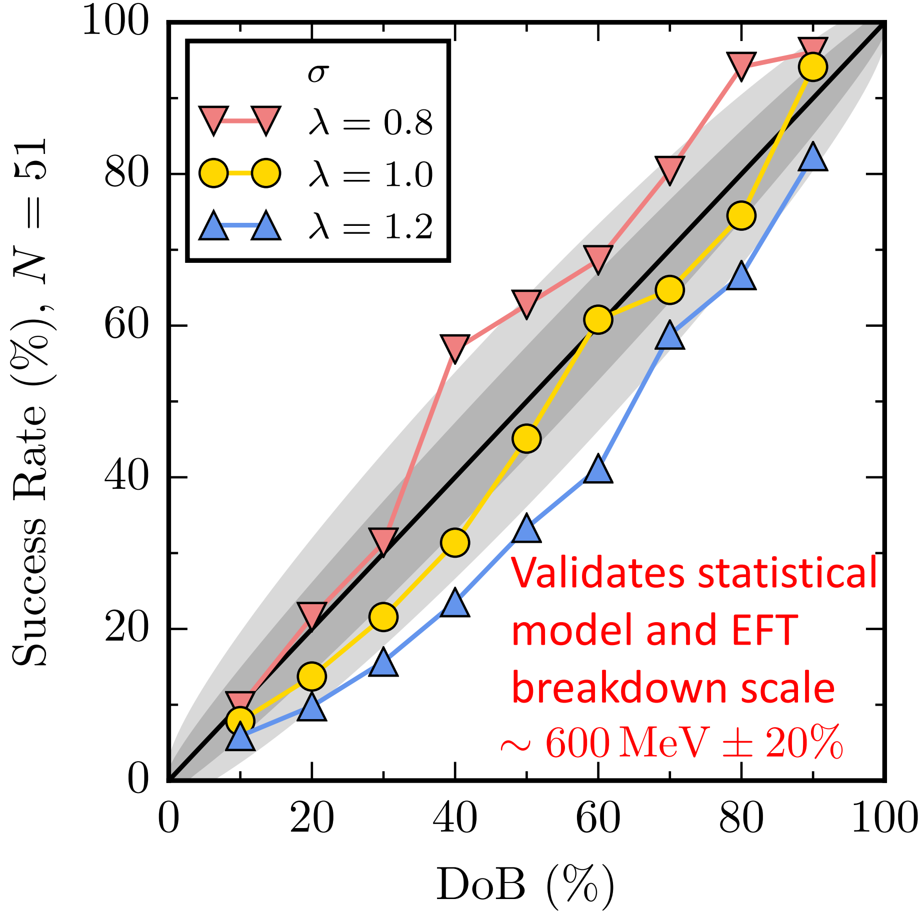

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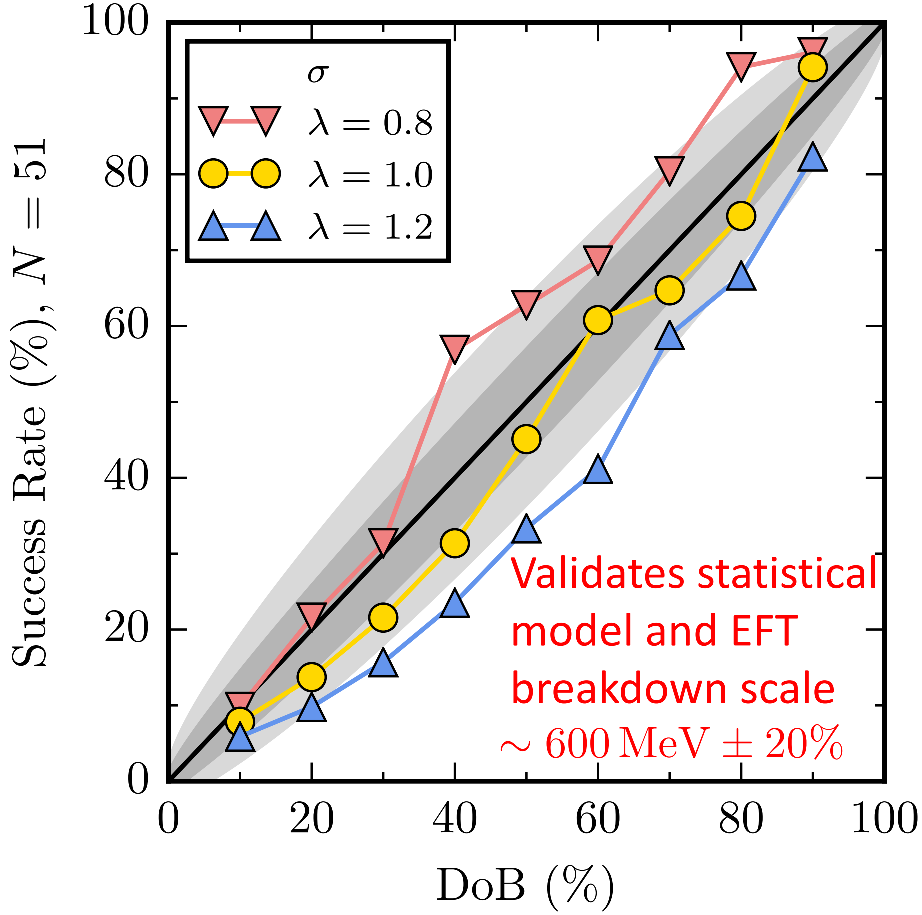

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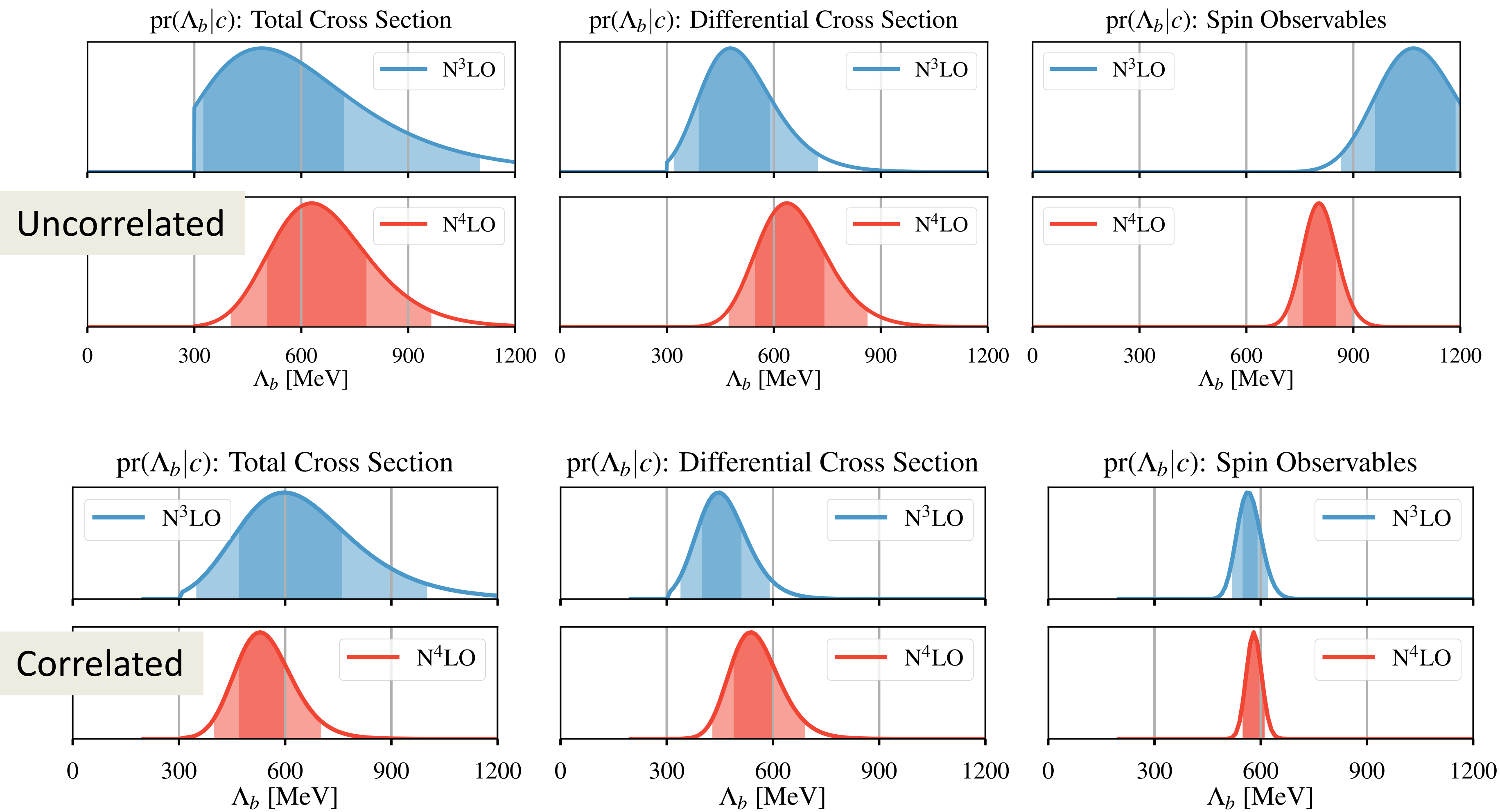
First time applied to effective field theories. What other model checking?

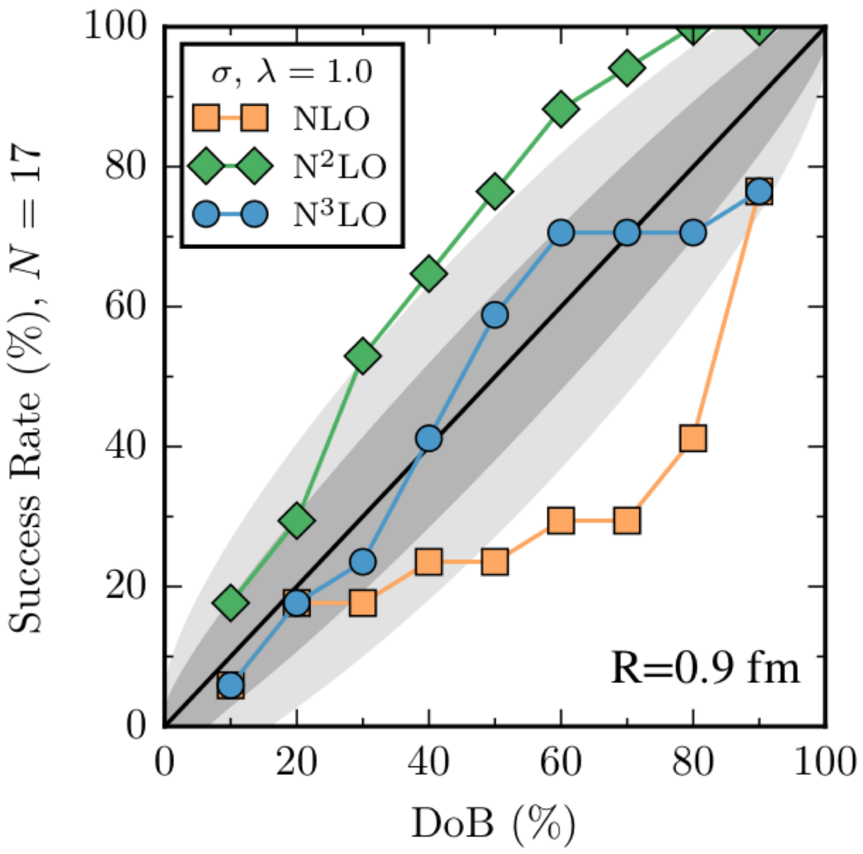
Physics discovery: What is the EFT breakdown scale?



- First extraction of EFT breakdown scale from convergence pattern
- Accounting for correlations with GP yields more consistent results

Bayesian Model Checking: identifying failures of *physics*

Melendez et al., PRC **96**, 024003 (2017)



- Compare two choices of regulator parameter R. Both give good fits to the NN data, but are they both behaving as expected from effective field theory?
- Look order-by-order for deviant behavior. R=0.9 fm looks ok.

Bayesian Model Checking: identifying failures of *physics*

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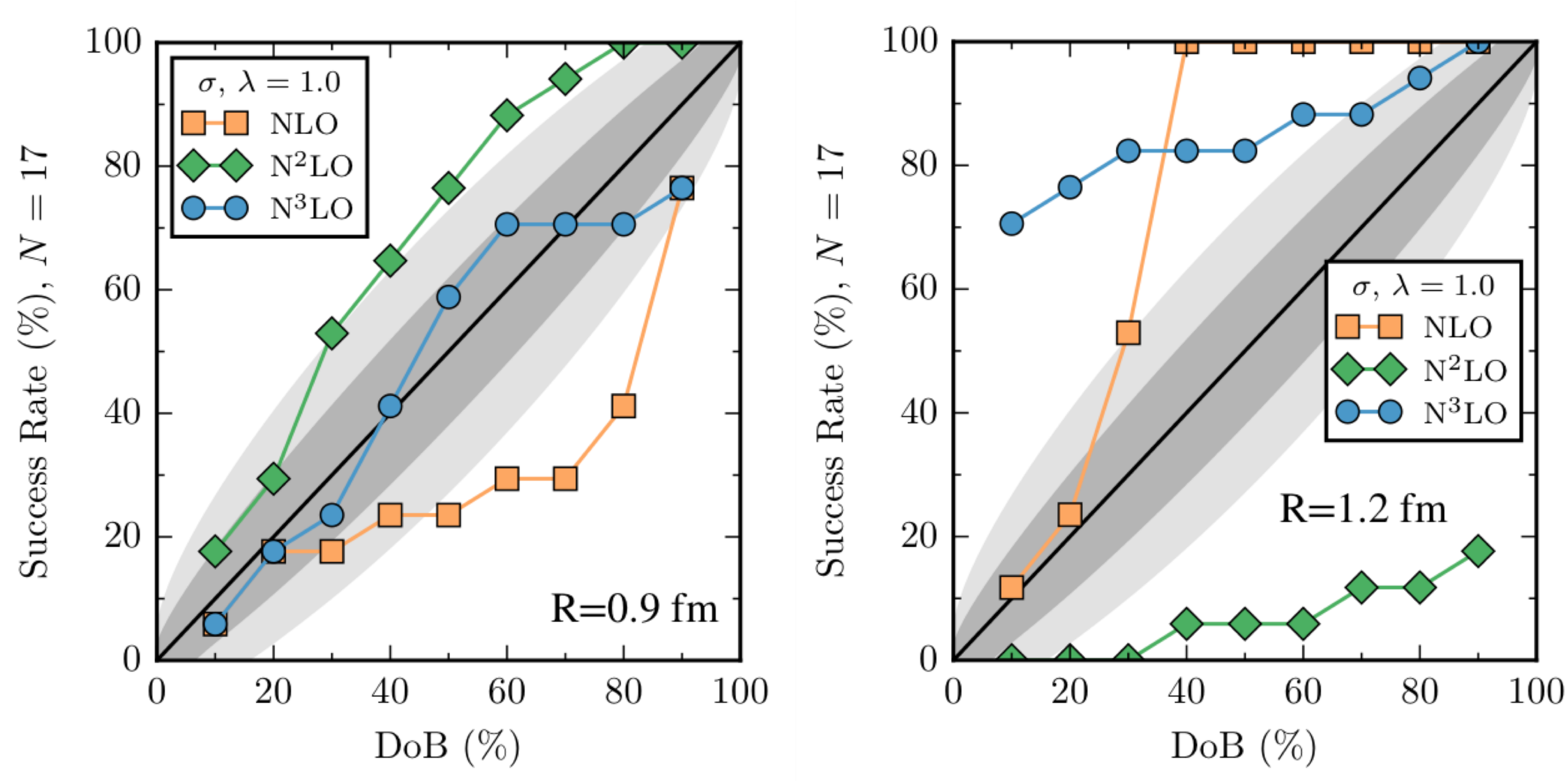

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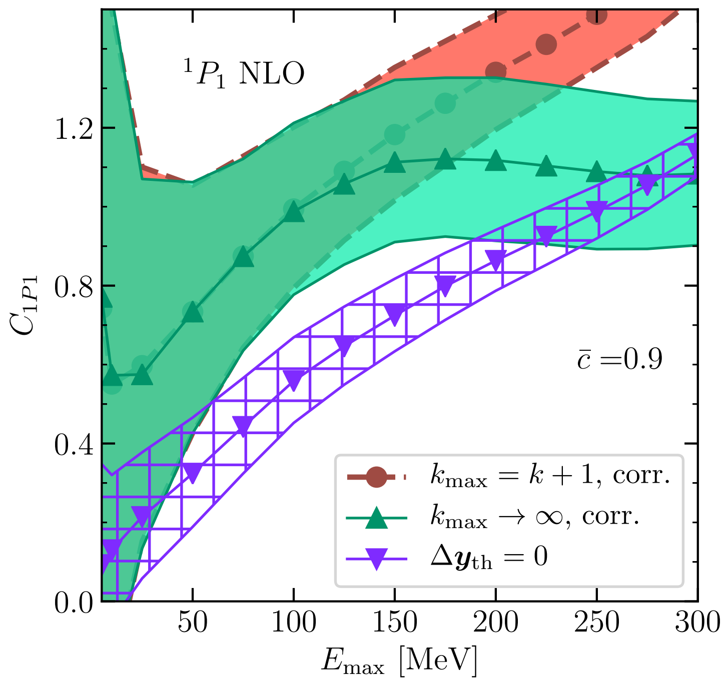
- Look order-by-order for deviant behavior. R=0.9 fm looks ok.
- But R=1.2 fm does not! ⇒ points to "regulator artifacts" that distort physics

How much data to use when fitting EFT parameters?

- An EFT calculation has smaller truncation errors at low energies but where to stop using data for parameter estimation?
- The $^1P_1$ example shows a least squares fit with no truncation error (purple triangles and band) shows no stability in the parameter value as a function of the maximum energy used.
- But our discrepancy model (green) generates a stable prediction with a more robust 68% band.



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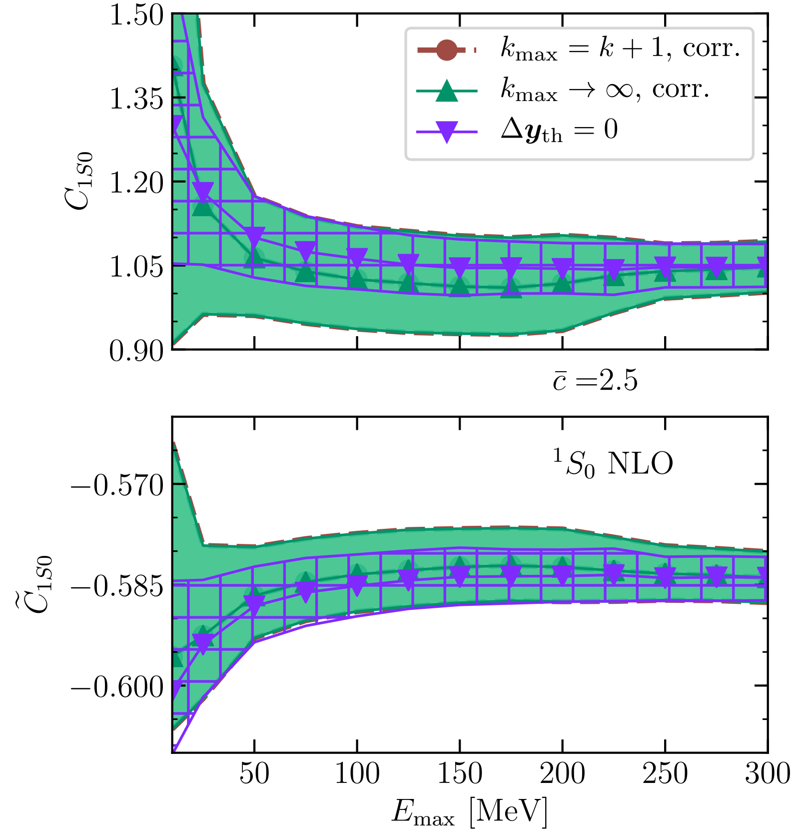
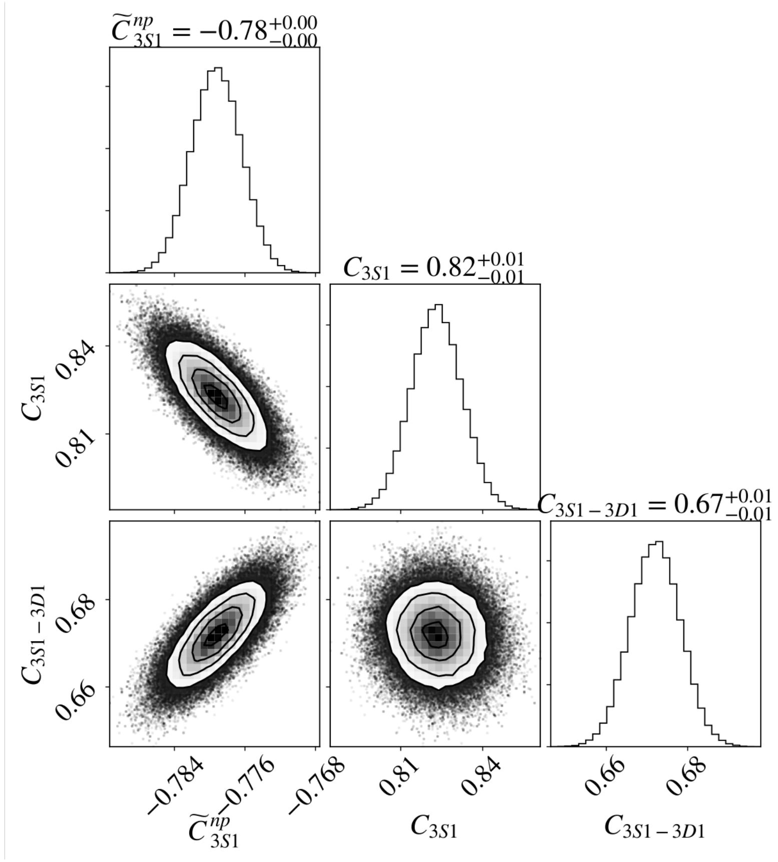
- The $^1S_0$ example shows that at high enough order, the parameters are well determined with or without the theory discrepancy model.



More physics discovery through statistics: Redundant operators

- One example (of many) of how statistical analysis has led to physics discover, here while doing parameter estimation
- Projected posterior plots for NN parameters generally are close to Gaussian.



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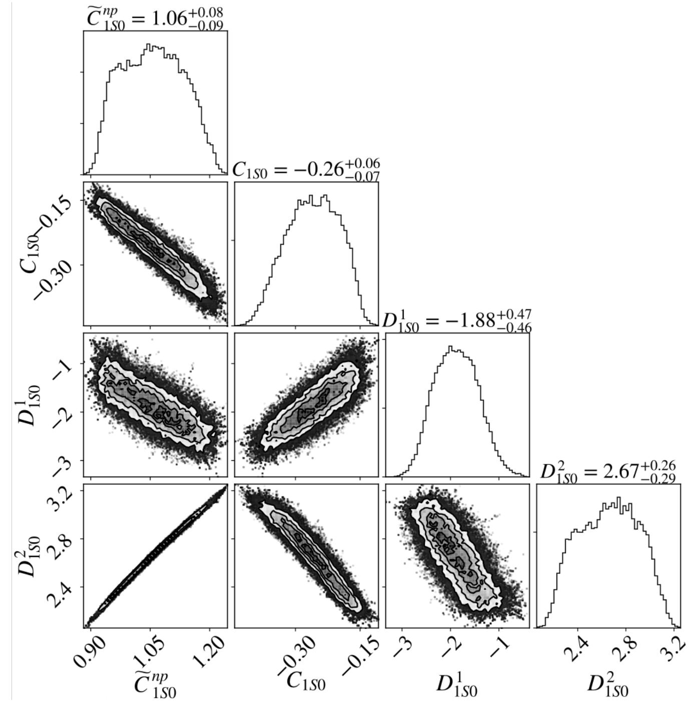

$$
\begin{aligned}
D^1_{(1S0)}p^2p'^2 + D^2_{(1S0)}(p^4+p'^4) \\
&= \frac{1}{4}(D^1_{(1S0)}+2D^2_{(1S0)})(p^2+p'^2)^2 \\
&\quad -\frac{1}{4}(D^1_{(1S0)}-2D^2_{(1S0)})(p^2-p'^2)^2 \\
&= (D^1_{(1S0)}+2D^2_{(1S0)})p^2p'^2 + D^2_{(1S0)}(p^2-p'^2)^2
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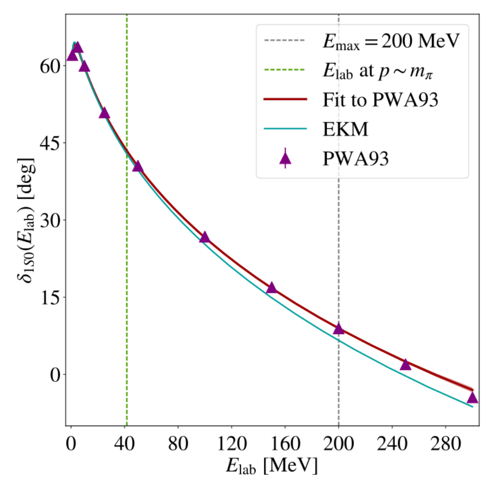
$$



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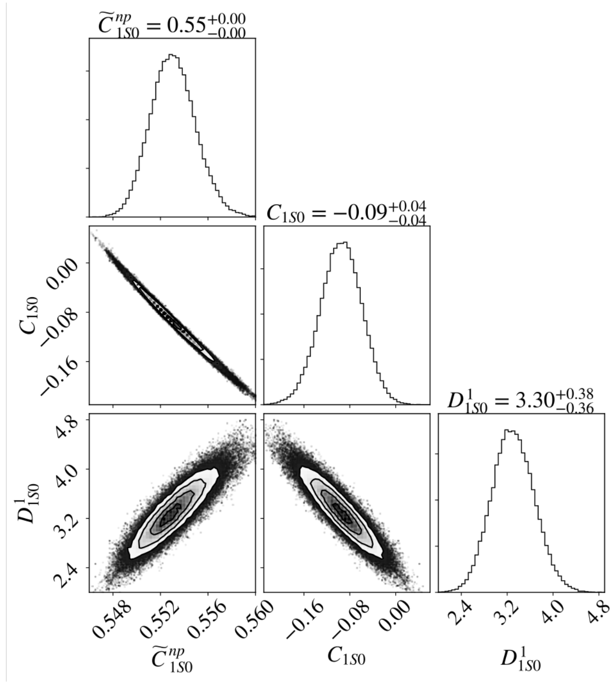
- When they are not, it is a signal to look for a physics reason. Led us to a redundancy, not noticed for 10 years!.
- Eliminating removes 3 of 15 parameters and leads to much better interactions!



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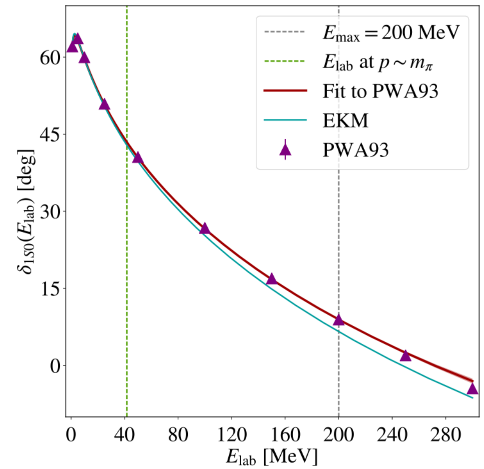
$$



Summary: Bayesian Statistics for EFTs

- In this era of precision nuclear physics, robust UQ for theoretical calculations has become essential, but development of appropriate tools is still in its infancy
- Bayesian statistical methods are particularly well suited for effective field theories
- Provides much more than just theoretical error bars ⇒ tools for physics discovery:
    - Is the effective field theory behaving as advertised? Is there systematic improvement at the predicted rate?
    - Identifies problematic implementations (e.g., are we dominated by regulator artifacts or are there redundant operators?)
    - Stimulates new ideas such as breakdown scales and correlation length in energy or angle and enables their extraction
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Many open problems to be addressed:

- Model selection opportunities still to be explored, e.g., which are the best degrees of freedom: nucleons + pions only, nucleons + deltas + pions, nucleons only, …
- Alternative model checking methods
- Parameter estimation with curve-wise discrepancy model
- Exploring the physics application of the GP hyperparameters
- Full propagation of uncertainties to very expensive many-body calculations
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Interactions with statisticians are invaluable!

Thank you!

Extra Slides

Some BUQEYE publications on UQ for EFT

- “A recipe for EFT uncertainty quantification in nuclear physics”, J. Phys. G 42, 034028 (2015)
- “Quantifying truncation errors in effective field theory”, Phys. Rev. C 92, 024005 (2015) [with Natalie Klco]
- “Bayesian parameter estimation for effective field theories”, J. Phys. G 43, 074001 (2016)
- “Bayesian truncation errors in chiral EFT: nucleon-nucleon observables”, Phys. Rev. C 96, 024003 (2017) [Editors’ Suggestion]
- “Exploring Bayesian parameter estimation for chiral effective field theory using nucleon-nucleon phase shifts” (2018) [just submitted to J. Phys. G]
- “A Gaussian Process Model for Continuous Truncation Errors in Effective Field Theories” [with M. Pratola; in preparation]

Discrepancy distribution

Remember the goal:

$$y_{\mathrm{exp}}(x) = y_{\mathrm{th}}(x, \vec{a}) + \delta y_{\mathrm{th}}(x) + \delta y_{\mathrm{exp}}$$

Our convergence assumptions

$$\mathrm{pr}(c_n \mid \boldsymbol{\theta}) \overset{\mathrm{iid}}{=} \mathcal{GP}(\mu, \sigma^2 R_\ell)$$

$$\delta y_{\mathrm{th}}(x) = y_{\mathrm{ref}} \sum_{n=k+1}^{\infty} c_n Q^n$$

Gaussian sum rules

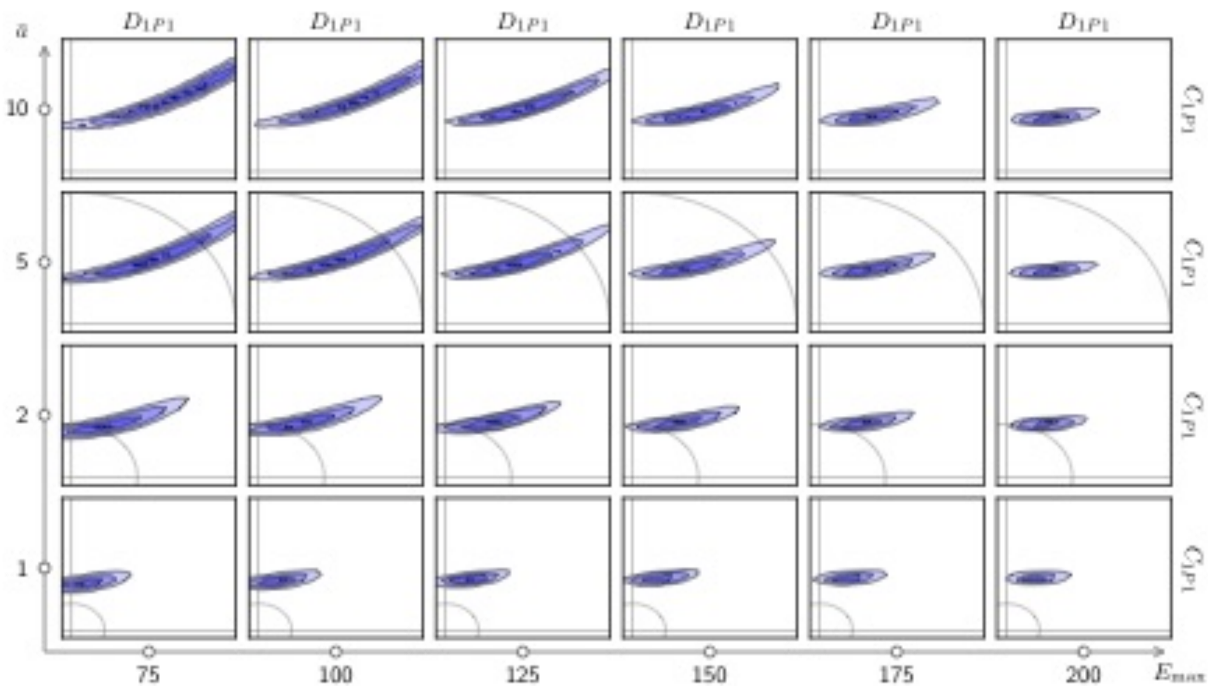
$$a\mathcal{N}(\mu_1, \Sigma_1) + b\mathcal{N}(\mu_2, \Sigma_2) = \mathcal{N}(a\mu_1 + b\mu_2, a^2\Sigma_1 + b^2\Sigma_2)$$

Discrepancy Distribution

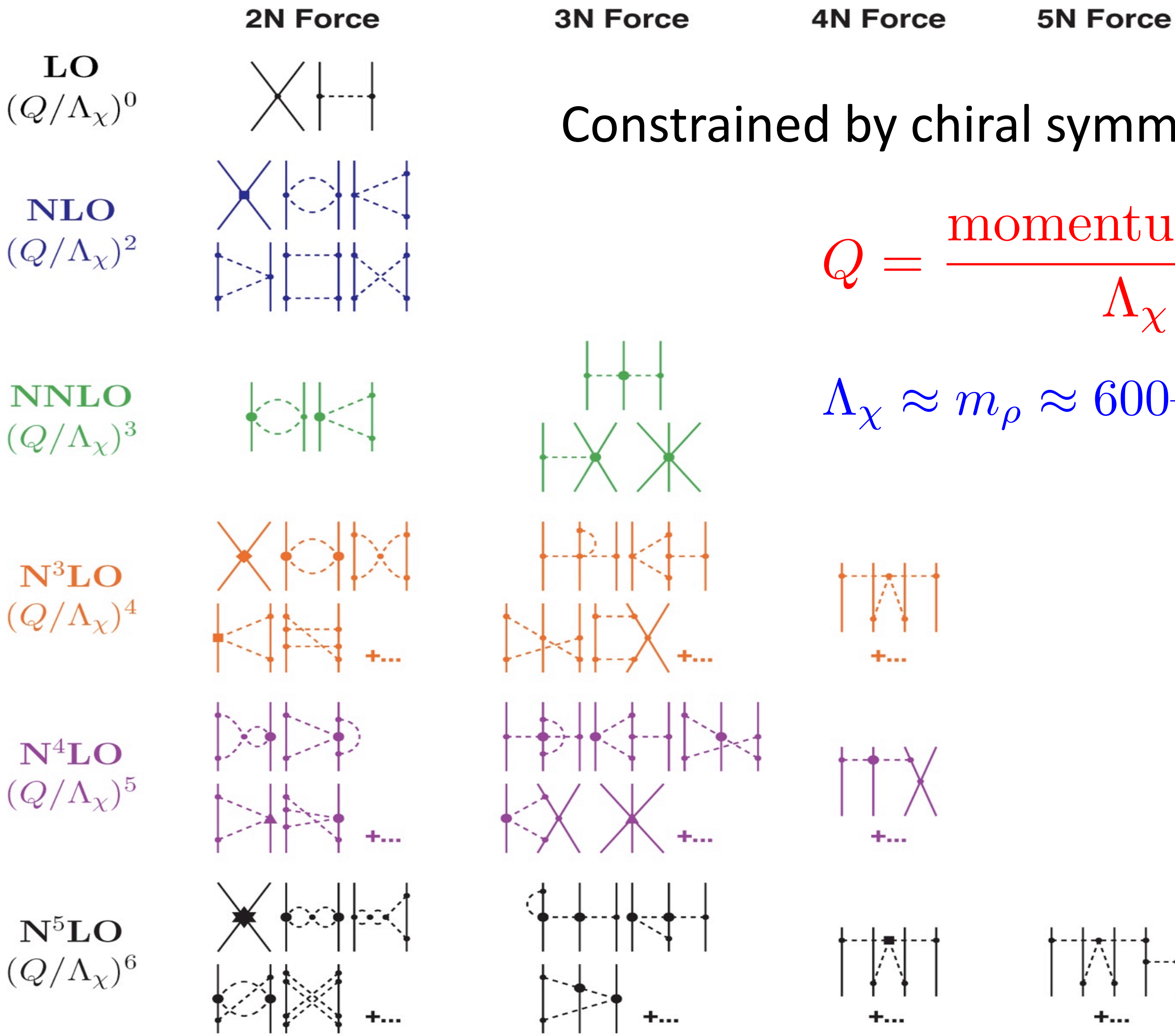
$$\mathrm{pr}(\delta y_{\mathrm{th}} \mid \boldsymbol{\theta}) = \mathcal{GP}\,(\mu_{\mathrm{th}}, \Sigma_{\mathrm{th}}) = \mathcal{GP}\left(\frac{\mu Q^{k+1}}{1-Q}, y_{\mathrm{ref}}^2 \frac{\sigma^2 Q^{2(k+1)}}{1-Q^2} R_\ell\right)$$

Importance of a prior for naturalness

$E_{\max}$ [MeV]	C_{1P1} $\bar{a}=1$	C_{1P1} $\bar{a}=2$	C_{1P1} $\bar{a}=5$	C_{1P1} $\bar{a}=10$	C_{1P1} $\bar{a}=20$	D_{1P1} $\bar{a}=1$	D_{1P1} $\bar{a}=2$	D_{1P1} $\bar{a}=5$	D_{1P1} $\bar{a}=10$	D_{1P1} $\bar{a}=20$
25	$1.5^{+0.2}_{-0.2}$	$1.7^{+0.5}_{-0.3}$	$2.4^{+2.2}_{-0.8}$	$5.2^{+6.1}_{-3.3}$	12^{+14}_{-8}	$0.0^{+0.9}_{-0.9}$	$0.5^{+1.6}_{-1.7}$	$2.5^{+3.2}_{-3.0}$	$6.3^{+4.8}_{-5.0}$	11^{+7}_{-7}
50	$1.7^{+0.2}_{-0.2}$	$1.9^{+0.6}_{-0.3}$	$2.8^{+2.1}_{-1.0}$	$5.4^{+5.7}_{-3.0}$	12^{+14}_{-8}	$0.1^{+0.8}_{-0.8}$	$0.9^{+1.5}_{-1.4}$	$3.2^{+2.9}_{-2.6}$	$6.6^{+4.5}_{-4.2}$	11^{+7}_{-7}
75	$1.8^{+0.2}_{-0.2}$	$2.0^{+0.5}_{-0.3}$	$3.0^{+2.0}_{-1.0}$	$4.6^{+5.0}_{-2.2}$	$8.5^{+12}_{-5.3}$	$0.4^{+0.8}_{-0.8}$	$1.3^{+1.3}_{-1.3}$	$3.5^{+2.7}_{-2.2}$	$5.8^{+4.4}_{-3.4}$	$9.4^{+6.9}_{-5.6}$
100	$1.9^{+0.2}_{-0.2}$	$2.1^{+0.5}_{-0.3}$	$2.7^{+1.5}_{-0.7}$	$3.6^{+3.2}_{-1.3}$	$4.4^{+7.0}_{-2.0}$	$0.6^{+0.7}_{-0.7}$	$1.5^{+1.2}_{-1.1}$	$3.2^{+2.3}_{-1.8}$	$4.6^{+3.6}_{-2.6}$	$5.8^{+6.0}_{-3.3}$
125	$1.9^{+0.2}_{-0.1}$	$2.1^{+0.4}_{-0.2}$	$2.4^{+0.9}_{-0.4}$	$2.6^{+1.3}_{-0.6}$	$2.8^{+1.8}_{-0.7}$	$0.8^{+0.7}_{-0.7}$	$1.6^{+1.1}_{-1.0}$	$2.6^{+1.8}_{-1.4}$	$3.1^{+2.3}_{-1.6}$	$3.3^{+2.8}_{-1.8}$
150	$2.0^{+0.2}_{-0.1}$	$2.1^{+0.3}_{-0.2}$	$2.2^{+0.5}_{-0.3}$	$2.3^{+0.6}_{-0.3}$	$2.3^{+0.6}_{-0.3}$	$0.9^{+0.6}_{-0.6}$	$1.5^{+1.0}_{-0.8}$	$2.1^{+1.3}_{-1.1}$	$2.2^{+1.5}_{-1.1}$	$2.3^{+1.5}_{-1.2}$
175	$2.0^{+0.1}_{-0.1}$	$2.1^{+0.2}_{-0.1}$	$2.1^{+0.3}_{-0.2}$	$2.1^{+0.3}_{-0.2}$	$2.1^{+0.3}_{-0.2}$	$0.9^{+0.6}_{-0.5}$	$1.4^{+0.8}_{-0.7}$	$1.7^{+1.0}_{-0.8}$	$1.8^{+1.0}_{-0.8}$	$1.7^{+1.1}_{-0.8}$
200	$2.0^{+0.1}_{-0.1}$	$2.0^{+0.1}_{-0.1}$	$2.0^{+0.2}_{-0.1}$	$2.0^{+0.2}_{-0.1}$	$2.0^{+0.2}_{-0.1}$	$0.9^{+0.5}_{-0.5}$	$1.2^{+0.7}_{-0.6}$	$1.4^{+0.7}_{-0.6}$	$1.4^{+0.8}_{-0.7}$	$1.4^{+0.8}_{-0.7}$



Chiral EFT expansion of neutron-proton force [from R. Machleidt]



Constrained by chiral symmetry

$$Q = \frac{\mathrm{momentum}, m_\pi}{\Lambda_\chi}$$

$$\Lambda_\chi \approx m_\rho \approx 600\text{–}700\,\mathrm{MeV}$$